The mechanism for the oxidation of fuel blends n-heptane/toluene, methyl hexanoat/ n-heptane/toluene and ethyl pentanoate / n-heptane/toluene.

The mechanism for the oxidation of fuel blend n-heptane/toluene

```
ELEMENTS
H O C N AR
END
SPECIES

! Biradicals :
B1O
B2CO
B3C
B4CH
B5CH2
B6CH2

! Primary molecules :
! Reactants:
C7H16-1
C8H18-1
H2
H2O
O2
H2O2
CH4
HCHO
CH3OH
CO2
CH3OOH
C2H2
C2H4Z
C2H6
CH2COZ
CH3CHO
C2H5OH
C2H3OH
C2H5OOH
CH3COOOH
C3H6Y
C3H8
C4H8Y
C4H10
C2H5CHO
C3H7OH
C2H6CO
C3H8CO
C4H6Z2
C2H3CHOZ
C7H16
C8H18
C5H10Z
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C7H14Z
C6H12Z
C7H14Y
C8H16Y
C8H16Z
C5H10Y
C4H10OL
C4H10O2P
C3H8O2P
C5H12
C5H10OA
C4H8OA
C5H12OL
C6H14

! Secondary molecules :
C6H12OA
C7H14OA
C9H18Z
C10H20Z
C13H26Z
C12H24Z
C11H22Z
C14H28Z
C8H16OA
C9H18OA
C12H24OA
C11H22OA
C10H20OA
C13H26OA
C3H6OLY
C3H6O2PY
C4H6OAY
C4H8OLY
C6H10Y2
C7H12Y2
C10H18Y2
C11H20Y2
C8H14Y2
C4H8O2PY
C5H8OAY
C5H10OLY
C12H22Y2
C9H16Y2
C7H14OLY
C7H14O2PY
C8H14OAY
C8H16OLY
C14H26Y2
C15H28Y2
C8H16O2PY
C9H16OAY
C9H18OLY
C16H30Y2

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C13H24Y2
C5H10O2PY
C6H10OAY
C6H12OLY
C4H6OKZ
C5H8OKZ
C6H10OKZ
C7H12OKZ

! Cyclic primary molecules :
C2H4OE#3

! Cyclic secondary molecules :
C3H6OE#3
C4H8OE#3
C5H10OE#3
C7H14OE#3
C6H12OE#3
C8H16OE#3
C9H18OE#3
C10H20OE#3
C13H26OE#3
C12H24OE#3
C11H22OE#3
C14H28OE#3

! Benzenic primary molecules :

! Free radicals :
R1H   !   .h
R2OH   !   .oh
R3OOH   !   .o/oh
R4CH3   !   .ch3
R5CHO   !   .ch//o
R6CH2OH   !   .ch2/oh
R7CH3O   !   .o/ch3
R8CH3OO   !   .o/o/ch3
R9C2H   !   .c///ch
R10C2H3V   !   .ch//ch2
R11C2H5   !   .ch2/ch3
R12CHCOZ   !   .ch//c//o
R13CH2CHO   !   .ch2/ch//o
R14CH3CO   !   .c(//o)/ch3
R15C2H5O   !   .o/ch2/ch3
R16C2H4OOH   !   .ch2/ch2/o/oh
R17C2H5OO   !   .o/o/ch2/ch3
R18CH3COOO   !   .o/o/c(//o)/ch3
R19C3H7   !   .ch2/ch2/ch3
R20C4H9   !   .ch2/ch2/ch2/ch3
R21CH3OCO   !   .c(//o)/o/ch3
!R22CO2H   !   .c(//o)/oh
!R23C2H3O2B   !   .ch2/c(//o)/oh
!R24C2H4OH   !   .ch2/ch2/oh
!R25C2H4OH   !   .ch(/oh)/ch3
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```
R23C2H4OH   !   c.h2-ch2-oh
R24C2H4OH   !   ch3-c.h-oh
R25C2H5CO   !   ch3-ch2-c.o

R26C7H15   !   .ch(/ch2/ch2/ch3)2
R27C7H15   !   .ch2/ch2/ch2/ch2/ch2/ch2/ch3
R28C7H15   !   .ch(/ch3)/ch2/ch2/ch2/ch2/ch3
R29C7H15   !   .ch(/ch2/ch3)/ch2/ch2/ch2/ch3
R30C8H17   !   .ch2/c(/ch3)2/ch2/ch(/ch3)2
R31C8H17   !   .ch2/ch(/ch3)/ch2/c(/ch3)3
R32C8H17   !   .c(/ch3)2/ch2/c(/ch3)3
R33C8H17   !   .ch(/ch(/ch3)2)/c(/ch3)3
R34C4H9   !   .ch(/ch3)/ch2/ch3
R35C5H11   !   .ch2/ch2/ch2/ch2/ch3
R36C4H9   !   .ch2/ch(/ch3)2
R37C5H11   !   .ch2/c(/ch3)3
R38C4H9   !   .c(/ch3)3
R39C5H11   !   .ch(/ch2/ch3)2
R40C5H11   !   .ch(/ch3)/ch2/ch2/ch3
R41C6H13   !   .ch2/ch2/ch2/ch2/ch2/ch3
R42C7H15   !   .c(/ch3)2/ch2/ch(/ch3)2
R43C3H7   !   .ch(/ch3)2
R44C7H15   !   .ch(/ch3)/ch2/c(/ch3)3
 !Cyclic free radicals:
 !Benzenic free radicals:

! lumped Free radicals :
RC3H5Y
RC4H7Y
RC3H5O
RC7H13Y
RC8H15Y
RC5H9Y
RC5H9O
RC4H7O
RC3H5O3
RC6H11O
RC7H13O
RC5H9O3
RC4H7O3
RC6H11O3
RC7H13O3
RC8H15O
RC9H17O
RC12H23O
RC11H21O
RC10H19O
RC13H25O
RC8H15O3
RC9H17O3
RC11H23
RC12H23O3
RC10H21
RC11H21O3
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RC9H19
RC10H19O3
RC12H25
RC13H25O3
RC6H11Y
! lumped Cyclic free radicals :

N2
AR

!!!!!!!!!!Espиces rajoutйes pour le mйca toluиne

aC3H4      !ch2//ch//ch2                          propadiene = allene
pC3H4      !ch///c/ch3                                 propyne
C4H2       !ch///c/c///ch                         butadiyne = diacetylene
C4H4       !ch2//ch/c///ch                        1-buten-3-yne ou vinyl
acetylene
C4H6-12          !ch2//c//ch/ch3                       1,2-butadiиne ou
mйthyl allиne
C4H6-1           !ch///c/ch2/ch3                       1-butyne
C4H6-2           !ch3/c///c/ch3                        2-butyne
iC4H8      !ch2//c(ch3)/ch3                 2methyl-propene
C5H8       !ex ch2//ch/ch2/ch//ch2          pentadiene
iC5H8      !ex ch3/c(ch3)//c//ch2
!iC5H10          !ex ch3/ch(ch3)/ch//ch2
!C5H10           !ex ch2//ch/ch2/ch2/ch3          pentene
C5H8#      !c(#1)h2/ch2/ch//ch/ch2/1        cyclopentene
C5H6#      !c(#1)h//ch/ch//ch/ch2/1         cyclopentadiene
C6H6#      !c(#1)h&ch&ch&ch&ch&ch&1         benzene
toluene          !c(#1)h&ch&ch&ch&ch&ch&1(/ch3)
MCP              !c(#1)h2/ch2/ch//ch/ch(/ch3)/1  methylcyclopentene
MCPD       !c(#1)h//ch/ch//ch/ch(/ch3)/1   methylcyclopentadiene
C5H4O#           !o//c(#1)/ch//ch/ch//ch/1
C3H2       !.ch//c//c(.)h
C2H4O#3    !c(#1)h2/o/ch2/1
C2H3CHO          !ch(//o)/ch//ch2                 2-propenal
cC3H4      !c(#1)h2/ch//ch/1                      cyclopropene
cC3H6      !c(#1)h2/ch2/ch2/1                     cyclopropane
tC4H4      !ch2//c//c//ch2                        1,2,3 butatriene
C6H2       !ch///c/c///c/c///ch             hexatriyne
cC4H6      !c(#1)h2/ch//ch/ch2/1                  cyclobutene
lC6H4      !ch///c/ch//ch/c///ch
!lC6H6           !ch2//ch/c///c/ch//ch2     !MF car n'intervient plus (une
rйaction)
lC6H8      !ch2//ch/ch//ch/ch//ch2
C6H8#      !c(#1)h2/ch//ch/ch2/ch//ch/1     cyclohexadiene
C6H10#           !c(#1)h2/ch//ch/ch2/ch2/ch2/1   cyclohexene
C8H10#           !c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1   cyclooctatriene
!Especes excitees
OHE
CHE
iC3H7      !.ch(/ch3)2
C3H3       !ch///c/ch2(.)
C3H5Y      !.ch2/ch//ch2
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```
tC3H5      !ch2//c(.)/ch3
sC3H5      !.ch//ch/ch3
nC4H3      !.ch//ch/c///ch
iC4H3      !ch2//c(.)/c///ch
nC4H5      !.ch//ch/ch//ch2
iC4H5      !ch2//c(.)/ch//ch2
C4H5-1s          !ch///c/ch(.)/ch3
C4H5-1p          !.ch2/ch2/c///ch
C4H5-2           !.ch2/c///c/ch3
lC6H5      !ch///c/ch//ch/ch//ch(.)
lC6H7      !ex .ch//ch/ch//ch/ch//ch2
!lC6H9           !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus (une
rйaction)
C6H4#      !.c(#1)&ch&ch&ch&ch&c(.)&1
C6H5#      !.c(#1)&ch&ch&ch&ch&ch&1
C6H7#      !.c(#1)h/ch//ch/ch2/ch//ch/1
C6H9Z#           !.c(#1)h/ch//ch/ch2/ch2/ch2/1
C4H7-1           !.ch2/ch2/ch//ch2
C4H7-2           !ch3/c(.)//ch/ch3
C4H7Y      !ch3/c(.)h/ch//ch2
C4H7T      !ch2//c(.)/ch2/ch3
iC4H7      !.ch//c(/ch3)2
C4H7V      !.c(/ch3)//ch/ch3
!C5H7Y           !ch2//ch/ch//ch/c(.)h2
!iC5H7Y          !ch2//c(/c(.)h2)/ch//ch2
C5H9Y      !ch2//ch/c(.)h/ch2/ch3
iC5H9      !.ch2/ch(/ch3)/ch//ch2
!iC5H9Y          !ch3/c(.)(/ch3)/ch//ch2
CH2CHCO          !.ch2/ch//c//o
cC3H3      !.c(#1)h/ch//ch/1
! MECHANISM OF BENZENE
! Molecules
C4H4O      !ch2//ch/ch//c//o                          vinylketene
!lC5H6           !ch///c/ch//ch/ch3                         !MF car
n'intervient plus (une rйaction)
C5H5OH#          !c(#1)h//ch/ch//ch/ch(/oh)/1          cyclopentadienol
C6H5OH#          !c(#1)h&ch&ch&ch&ch&c(/oh)&1          phйnol
OC6H4O           !o//c(#1)/ch//ch/ch//ch/c(//o)/1      orthobenzoquinone
C6H5#C2H   !ch///c/c(#1)&ch&ch&ch&ch&ch/&1       phenylacetylene
etC6H5           !c(#1)h&ch&ch&ch&ch&c(/ch2/ch3)&1     ethylbenzene
styrene          !c(#1)h&ch&ch&ch&ch&c(/ch//ch2)&1
!C6H5C3H3  !c(#1)h&ch&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus
(une rйaction)
C10H10#          !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1  !
bicyclopentadienyl
C6H5CHO          !c(#1)h&ch&ch&ch&ch&c(/ch//o)&1       benzaldehyde
biphenyl   !c(#1)h&ch&ch&ch&ch&c(/c(#2)h&ch&ch&ch&ch&c&2)&1
C6H5OOH

! Radicals
C5H5#      !c(#1)(.)h/ch//ch/ch//ch/1
lC5H5      !.c///c/ch//ch/ch3
C5H3O#           !.c(#1)//ch/ch//ch/c(//o)&1
C5H5O#           !c(#1)h//ch/ch//ch/ch(/o(.))&1
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```
C5H4OH#         !.c(#1)//ch/ch//ch/ch(/oh)&1
C6H5O#          !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5O2          !.c(#1)&ch&ch&ch&ch&c(/o/o(.))&1
C6H4OH#         !.c(#1)&ch&ch&ch&ch&c(/oh)&1
OC6H4OH         !c(#1)h&ch&ch&ch&ch(/o(.))&c(/oh)&1


!MECHANISM OF TOLUENE
HOC6H4CH3  !oh/c(#1)&ch&ch&ch&ch&c(/ch3)&1 cresol
C6H4OHCHO  !oh/c(#1)&ch&ch&ch&ch&c(/ch//o)&1
C6H5CH2OH  !c(#1)h&ch&ch&ch&ch&c(/ch2/oh)&1
C6H5CH2OOH !c(#1)h&ch&ch&ch&ch&c(/ch2/o/oh)&1
bibenzyl   !ok
stilbene   !ok
benzyl          !c(#1)h&ch&ch&ch&ch&c(/c(.)h2)&1
C6H4CH3         !c(#1)h&ch&ch&ch&ch&c(/ch3)&1
C6H4OHCO   !oh/c(#1)&ch&ch&ch&ch&c(/c(.)//o)&1
HOC6H4CH2OO !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o/o(.))&1
OC6H4CH3   !o(.)/c(#1)&ch&ch&ch&ch&c(/ch3)&1
HOC6H4CH2  !oh/c(#1)&ch&ch&ch&ch&c(/c(.)h2)&1
C6H5CO          !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5CHOH   !c(#1)h&ch&ch&ch&ch&c(/c(.)h/oh)&1
C6H5CH2O   !c(#1)h&ch&ch&ch&ch&c(/ch2/o(.))&1
HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o(.))&1
C6H5CH2OO  !c(#1)h&ch&ch&ch&ch&c(/ch2/o/o(.))&1
C8H9#      !c(#1)h&ch&ch&ch&ch&c(/c(.)h2/ch2)&1
C8H9#-1         !c(#1)h&ch&ch&ch&ch&c(/ch2/c(.)h2)&1
C6H5C2H2   !c(#1)h&ch&ch&ch&ch&c(/ch//c(.)h)&1
C14H13#         !bibenzyl -H



!MECHANISM OF CYCLOPENTENE!
!C5H8-12        !ch2//c//ch/ch2/ch3
!C5H7#          !.c(#1)h/ch2/ch//ch/ch2/1
!C5H7#Y         !c(#1)h2/c(.)h/ch//ch/ch2/1
!C5H7#V         !c(#1)h2/ch2/c(.)//ch/ch2/1
!C5H7-1s        !ch(.)//ch/ch2/ch//ch2
!C5H7-2t        !ch2//ch/ch2/c(.)//ch2
!C5H7-4t        !ch3/c(.)//ch/ch//ch2
!C5H7-3t        !ch3/ch//c(.)/ch//ch2
!C5H7-5p        !ch2(.)/ch2/ch2/c///ch
!C5H7-12-5p     !ch2(.)/ch2/ch//c//ch2
!C5H9#          !.c(#1)h/ch2/ch2/ch2/ch2/1
!C5H9      !(.)ch2/ch2/ch2/ch//ch2
!RMCP1          !c(#1)h(.)/ch2/ch//ch/ch(/ch3)/1
!RMCP2          !c(#1)h2/ch2/ch//ch/ch(/ch2(.))/1
!RMCPY1         !c(#1)h2/ch(.)/ch//ch/ch(/ch3)/1
!RMCPY2         !c(#1)h2/ch2/ch//ch/c(.)(/ch3)/1
!RMCPD          !c(#1)h//ch/ch//ch/ch(/ch2(.))/1
!RMCPDY         !c(#1)h//ch/ch//ch/c(.)(/ch3)/1

!*Especes ajoutйes*!
!mfC5H5C2H2     !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1
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!C5H4CCH2  !c(#1)h//ch/ch//ch/c(//c//ch2)/1
!C5H5CCH   !c(#1)h//ch/ch//ch/ch(/c///ch)/1
!C6H5COCH3 !C6H5x/CO/CH3
C8H9#OOH   !C6H5#ch(/ooh)/ch3 ! c(#1)h&ch&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1
C8H9#O          !C6H5#ch(/o(.))/ch3 !
c(#1)h&ch&ch&ch&ch&c(/ch(/o(.))/ch3)&1
OOC6H4CH3  !o(.)/o/c(#1)&ch&ch&ch&ch&c(/ch3)&1
!C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!TolOCH2C6H5  !ch3/c(#1)&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolCH2bz     !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
CH3bzOHCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!Benzaldtol      !
c(#1)h&ch&ch&ch&ch&c(/c(//o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1
!HOC6H4CHO  !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1
!C6H5C4H7   !c(#1)h&ch&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1
naphthalene
!benzofuran
C8H8O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2
C8H7O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch(.)/ch2/2
C8H7O#-1        ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch(.)/2
naphthyl
indenyl
indene
!cumene
!CH3styre
C9H11#-1
C2H3C6H4CH2
!phenanthrene
!C6H5CH2CHO
!!!!!!!!!!!!!!!!!!!!!!!!
*********************************************************************
END


REACTIONS
!(k = A T**b exp(-E/RT)) A units: mole-cm-sec-K, E units cal/mole)

!     -----------------
!     PRIMARY REACTIONS
!     -----------------
!   molecular elimination :
!   unimolecular initiations :
C7H16-1=>R19C3H7+R20C4H9    2.0E+0017  0.000  85750.3  ! UI 1 KB
C7H16-1=>R11C2H5+R35C5H11    1.6E+0017  0.000  85815.5  ! UI 2 KB
C7H16-1=>R4CH3+R41C6H13    3.2E+0017  0.000  87654.8  ! UI 3 KB
C8H18-1=>R4CH3+R42C7H15    1.2E+0018  0.000  81845.9  ! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9    2.4E+0017  0.000  78804.1  ! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11    4.6E+0017  0.000  83562.0  ! UI 6 KB
C8H18-1=>R4CH3+R44C7H15    8.0E+0017  0.000  87665.1  ! UI 7 KB

!   bimolecular initiations :
C7H16-1+O2=>R3OOH+R26C7H15    1.4E+0013  0.000  50652.5  ! BI 8 CN
C7H16-1+O2=>R3OOH+R27C7H15    4.2E+0013  0.000  53033.1  ! BI 9 CN
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C7H16-1+O2=>R3OOH+R28C7H15    2.8E+0013  0.000  50588.2  ! BI 10 CN
C7H16-1+O2=>R3OOH+R29C7H15    2.8E+0013  0.000  50652.5  ! BI 11 CN
C8H18-1+O2=>R3OOH+R30C8H17    6.3E+0013  0.000  53033.0  ! BI 12 CN
C8H18-1+O2=>R3OOH+R31C8H17    4.2E+0013  0.000  52333.1  ! BI 13 CN
C8H18-1+O2=>R3OOH+R32C8H17    7.0E+0012  0.000  47243.3  ! BI 14 CN
C8H18-1+O2=>R3OOH+R33C8H17    1.4E+0013  0.000  50652.7  ! BI 15 CN

!   additions :

!   additions with oxygen:

!   isomerisations :
R20C4H9=R34C4H9    3.3E+0009  1.000  37000.0  ! IS 16 KB
R26C7H15=R28C7H15    6.7E+0009  1.000  37000.0  ! IS 17 KB
R26C7H15=R27C7H15    1.7E+0009  1.000  19800.0  ! IS 18 KB
R27C7H15=R29C7H15    9.9E+0007  1.000  37000.0  ! IS 19 KB
R27C7H15=R28C7H15    1.7E+0007  1.000  17400.0  ! IS 20 KB
R28C7H15=R29C7H15    5.7E+0008  1.000  17300.0  ! IS 21 KB
R30C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 22 KB
R30C8H17=R32C8H17    2.9E+0008  1.000  15300.0  ! IS 23 KB
R30C8H17=R31C8H17    3.0E+0008  1.000  14500.0  ! IS 24 KB
R31C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 25 KB
R35C5H11=R39C5H11    3.3E+0009  1.000  37000.0  ! IS 26 KB
R35C5H11=R40C5H11    5.7E+0008  1.000  17300.0  ! IS 27 KB

!   Decomposition of OOQOOH into branching agents:

!   beta-scissions :
R19C3H7=>R4CH3+C2H4Z    2.0E+0013  0.000  31000.0  ! DE 28 CN
R19C3H7=>R1H+C3H6Y    3.0E+0013  0.000  38000.0  ! DE 29 CN
R20C4H9=>R11C2H5+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 30 CW
R20C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 31 CN
R26C7H15=>R11C2H5+C5H10Z    4.0E+0013  0.000  28700.0  ! DE 32 CW
R26C7H15=>R1H+C7H14Z    6.0E+0013  0.000  38000.0  ! DE 33 CN
R27C7H15=>R35C5H11+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 34 CW
R27C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 35 CN
R28C7H15=>R20C4H9+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 36 CW
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 37 CN
     DUPLICATE
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 38 CN
     DUPLICATE
R29C7H15=>R19C3H7+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 39 CW
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 40 CN
     DUPLICATE
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 41 CN
     DUPLICATE
R29C7H15=>R4CH3+C6H12Z    2.0E+0013  0.000  31000.0  ! DE 42 CN
R30C8H17=>R36C4H9+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 43 CW
R30C8H17=>R4CH3+C7H14Y    4.0E+0013  0.000  31000.0  ! DE 44 CN
R31C8H17=>R37C5H11+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 45 CW
R31C8H17=>R4CH3+C7H14Z    2.0E+0013  0.000  31000.0  ! DE 46 CN
R31C8H17=>R1H+C8H16Y    1.5E+0013  0.000  37500.0  ! DE 47 CN
R32C8H17=>R38C4H9+C4H8Y    2.0E+0013  0.000  26700.0  ! DE 48
R32C8H17=>R1H+C8H16Y    6.0E+0013  0.000  39000.0  ! DE 49 CN
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R32C8H17=>R1H+C8H16Z    3.0E+0013  0.000  38000.0  ! DE 50 CN
R33C8H17=>R4CH3+C7H14Z    4.0E+0013  0.000  31000.0  ! DE 51 CN
R33C8H17=>R4CH3+C7H14Y    6.0E+0013  0.000  31000.0  ! DE 52 CN
R33C8H17=>R1H+C8H16Z    3.0E+0013  0.000  37500.0  ! DE 53 CN
R34C4H9=>R4CH3+C3H6Y    2.0E+0013  0.000  31000.0  ! DE 54 CN
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 55 CN
     DUPLICATE
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  39000.0  ! DE 56 CN
     DUPLICATE
R35C5H11=>R19C3H7+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 57 CW
R35C5H11=>R1H+C5H10Z    3.0E+0013  0.000  38000.0  ! DE 58 CN
R36C4H9=>R4CH3+C3H6Y    4.0E+0013  0.000  31000.0  ! DE 59 CN
R36C4H9=>R1H+C4H8Y    3.0E+0013  0.000  37500.0  ! DE 60 CN
R37C5H11=>R4CH3+C4H8Y    6.0E+0013  0.000  31000.0  ! DE 61 CN
R38C4H9=>R1H+C4H8Y    9.0E+0013  0.000  39000.0  ! DE 62 CN
R39C5H11=>R4CH3+C4H8Y    4.0E+0013  0.000  31000.0  ! DE 63 CN
R39C5H11=>R1H+C5H10Y    6.0E+0013  0.000  38000.0  ! DE 64 CN
R40C5H11=>R11C2H5+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 65 CW
R40C5H11=>R1H+C5H10Z    3.0E+0013  0.000  39000.0  ! DE 66 CN
R40C5H11=>R1H+C5H10Y    3.0E+0013  0.000  38000.0  ! DE 67 CN
R41C6H13=>R20C4H9+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 68 CW
R41C6H13=>R1H+C6H12Z    3.0E+0013  0.000  38000.0  ! DE 69 CN
R42C7H15=>R43C3H7+C4H8Y    2.0E+0013  0.000  27700.0  ! DE 70
R42C7H15=>R1H+C7H14Y    3.0E+0013  0.000  38000.0  ! DE 71 CN
     DUPLICATE
R42C7H15=>R1H+C7H14Y    6.0E+0013  0.000  39000.0  ! DE 72 CN
     DUPLICATE
R43C3H7=>R1H+C3H6Y    6.0E+0013  0.000  39000.0  ! DE 73 CN
R44C7H15=>R38C4H9+C3H6Y    2.0E+0013  0.000  26700.0  ! DE 74
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 75 CN
     DUPLICATE
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 76 CN
     DUPLICATE
! decomposition of R(.)CO free radicals

!   decomposition to o-rings :

!   oxidations :
R26C7H15+O2=>C7H14Z+R3OOH    3.9E+0012  0.000  5000.0  ! OX 77 CN
R27C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 78 CN
R28C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 79 CN
     DUPLICATE
R28C7H15+O2=>C7H14Z+R3OOH    8.1E+0011  0.000  5000.0  ! OX 80 CN
     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 81 CN
     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 82 CN
     DUPLICATE
R31C8H17+O2=>C8H16Y+R3OOH    6.4E+0011  0.000  5000.0  ! OX 83 CN
R32C8H17+O2=>C8H16Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 84 CN
R32C8H17+O2=>C8H16Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 85 CN
R33C8H17+O2=>C8H16Z+R3OOH    6.4E+0011  0.000  5000.0  ! OX 86 CN
R38C4H9+O2=>C4H8Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 87 CW
R43C3H7+O2=>C3H6Y+R3OOH    2.3E+0012  0.000  5000.0  ! OX 88 CW
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!   oxidations of R(.)(OH) radicals:

!   metathesis :
B1O+C7H16-1=>R2OH+R26C7H15    2.6E+0013  0.000  5200.0  ! ME 89 CW
B1O+C7H16-1=>R2OH+R27C7H15    1.0E+0014  0.000  7850.0  ! ME 90 CW
B1O+C7H16-1=>R2OH+R28C7H15    5.2E+0013  0.000  5200.0  ! ME 91 CW
B1O+C7H16-1=>R2OH+R29C7H15    5.2E+0013  0.000  5200.0  ! ME 92 CW
B1O+C8H18-1=>R2OH+R30C8H17    1.5E+0014  0.000  7850.0  ! ME 93 CW
B1O+C8H18-1=>R2OH+R31C8H17    1.0E+0014  0.000  7850.0  ! ME 94 CW
B1O+C8H18-1=>R2OH+R32C8H17    1.0E+0013  0.000  3280.0  ! ME 95 CW
B1O+C8H18-1=>R2OH+R33C8H17    2.6E+0013  0.000  5200.0  ! ME 96 CW
C7H16-1+R1H=>H2+R26C7H15    9.0E+0006  2.000  5000.0  ! ME 97 CW
C7H16-1+R1H=>H2+R27C7H15    5.7E+0007  2.000  7700.0  ! ME 98 CW
C7H16-1+R1H=>H2+R28C7H15    1.8E+0007  2.000  5000.0  ! ME 99 CW
C7H16-1+R1H=>H2+R29C7H15    1.8E+0007  2.000  5000.0  ! ME 100 CW
C8H18-1+R1H=>H2+R30C8H17    8.6E+0007  2.000  7700.0  ! ME 101 CW
C8H18-1+R1H=>H2+R31C8H17    5.7E+0007  2.000  7700.0  ! ME 102 CW
C8H18-1+R1H=>H2+R32C8H17    4.2E+0006  2.000  2400.0  ! ME 103 CN
C8H18-1+R1H=>H2+R33C8H17    9.0E+0006  2.000  5000.0  ! ME 104 CW
C7H16-1+R2OH=>H2O+R26C7H15    2.6E+0006  2.000  -765.0  ! ME 105 CW
C7H16-1+R2OH=>H2O+R27C7H15    5.4E+0006  2.000  450.0  ! ME 106 CW
C7H16-1+R2OH=>H2O+R28C7H15    5.2E+0006  2.000  -765.0  ! ME 107 CW
C7H16-1+R2OH=>H2O+R29C7H15    5.2E+0006  2.000  -765.0  ! ME 108 CW
C8H18-1+R2OH=>H2O+R30C8H17    8.1E+0006  2.000  450.0  ! ME 109 CW
C8H18-1+R2OH=>H2O+R31C8H17    5.4E+0006  2.000  450.0  ! ME 110 CW
C8H18-1+R2OH=>H2O+R32C8H17    1.1E+0006  2.000  -1865.0  ! ME 111 CW
C8H18-1+R2OH=>H2O+R33C8H17    2.6E+0006  2.000  -765.0  ! ME 112 CW
C7H16-1+R3OOH=>H2O2+R26C7H15    4.0E+0011  0.000  15500.0  ! ME 113 CN
C7H16-1+R3OOH=>H2O2+R27C7H15    1.2E+0012  0.000  17000.0  ! ME 114 CN
C7H16-1+R3OOH=>H2O2+R28C7H15    8.0E+0011  0.000  15500.0  ! ME 115 CN
C7H16-1+R3OOH=>H2O2+R29C7H15    8.0E+0011  0.000  15500.0  ! ME 116 CN
C8H18-1+R3OOH=>H2O2+R30C8H17    1.8E+0012  0.000  17000.0  ! ME 117 CN
C8H18-1+R3OOH=>H2O2+R31C8H17    1.2E+0012  0.000  17000.0  ! ME 118 CN
C8H18-1+R3OOH=>H2O2+R32C8H17    2.0E+0011  0.000  14000.0  ! ME 119 CN
C8H18-1+R3OOH=>H2O2+R33C8H17    4.0E+0011  0.000  15500.0  ! ME 120 CN
C7H16-1+R4CH3=>CH4+R26C7H15    2.0E+0011  0.000  9600.0  ! ME 121 CN
C7H16-1+R4CH3=>CH4+R27C7H15    6.0E-0001  4.000  8200.0  ! ME 122 CN
C7H16-1+R4CH3=>CH4+R28C7H15    4.0E+0011  0.000  9600.0  ! ME 123 CN
C7H16-1+R4CH3=>CH4+R29C7H15    4.0E+0011  0.000  9600.0  ! ME 124 CN
C8H18-1+R4CH3=>CH4+R30C8H17    9.0E-0001  4.000  8200.0  ! ME 125 CN
C8H18-1+R4CH3=>CH4+R31C8H17    6.0E-0001  4.000  8200.0  ! ME 126 CN
C8H18-1+R4CH3=>CH4+R32C8H17    1.0E+0011  0.000  7900.0  ! ME 127 CW
C8H18-1+R4CH3=>CH4+R33C8H17    2.0E+0011  0.000  9600.0  ! ME 128 CN
C7H16-1+R5CHO=>HCHO+R26C7H15    1.0E+0007  1.900  17000.0  ! ME 129 CN
C7H16-1+R5CHO=>HCHO+R27C7H15    2.0E+0005  2.500  18500.0  ! ME 130 CN
C7H16-1+R5CHO=>HCHO+R28C7H15    2.2E+0007  1.900  17000.0  ! ME 131 CN
C7H16-1+R5CHO=>HCHO+R29C7H15    2.2E+0007  1.900  17000.0  ! ME 132 CN
C8H18-1+R5CHO=>HCHO+R30C8H17    3.1E+0005  2.500  18500.0  ! ME 133 CN
C8H18-1+R5CHO=>HCHO+R31C8H17    2.0E+0005  2.500  18500.0  ! ME 134 CN
C8H18-1+R5CHO=>HCHO+R32C8H17    3.4E+0004  2.500  13500.0  ! ME 135 CN
C8H18-1+R5CHO=>HCHO+R33C8H17    1.0E+0007  1.900  17000.0  ! ME 136 CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15    6.0E+0001  2.950  12000.0  ! ME 137 CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15    2.0E+0002  2.950  14000.0  ! ME 138 CN
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C7H16-1+R6CH2OH=>CH3OH+R28C7H15    1.2E+0002  2.950  12000.0  ! ME 139 CN
C7H16-1+R6CH2OH=>CH3OH+R29C7H15    1.2E+0002  2.950  12000.0  ! ME 140 CN
C8H18-1+R6CH2OH=>CH3OH+R30C8H17    3.0E+0002  2.950  14000.0  ! ME 141 CN
C8H18-1+R6CH2OH=>CH3OH+R31C8H17    2.0E+0002  2.950  14000.0  ! ME 142 CN
C8H18-1+R6CH2OH=>CH3OH+R32C8H17    1.2E+0002  2.760  10800.0  ! ME 143 CN
C8H18-1+R6CH2OH=>CH3OH+R33C8H17    6.0E+0001  2.950  12000.0  ! ME 144 CN
C7H16-1+R7CH3O=>CH3OH+R26C7H15    1.5E+0011  0.000  4500.0  ! ME 145 CN
C7H16-1+R7CH3O=>CH3OH+R27C7H15    3.2E+0011  0.000  7300.0  ! ME 146 CN
C7H16-1+R7CH3O=>CH3OH+R28C7H15    2.9E+0011  0.000  4500.0  ! ME 147 CN
C7H16-1+R7CH3O=>CH3OH+R29C7H15    2.9E+0011  0.000  4500.0  ! ME 148 CN
C8H18-1+R7CH3O=>CH3OH+R30C8H17    4.9E+0011  0.000  7300.0  ! ME 149 CN
C8H18-1+R7CH3O=>CH3OH+R31C8H17    3.2E+0011  0.000  7300.0  ! ME 150 CN
C8H18-1+R7CH3O=>CH3OH+R32C8H17    2.3E+0010  0.000  2900.0  ! ME 151 CN
C8H18-1+R7CH3O=>CH3OH+R33C8H17    1.5E+0011  0.000  4500.0  ! ME 152 CN
C7H16-1+R8CH3OO=>CH3OOH+R26C7H15    3.0E+0012  0.000  17500.0  ! ME 153
CN
C7H16-1+R8CH3OO=>CH3OOH+R27C7H15    1.2E+0013  0.000  20000.0  ! ME 154
CN
C7H16-1+R8CH3OO=>CH3OOH+R28C7H15    6.0E+0012  0.000  17500.0  ! ME 155
CN
C7H16-1+R8CH3OO=>CH3OOH+R29C7H15    6.0E+0012  0.000  17500.0  ! ME 156
CN
C8H18-1+R8CH3OO=>CH3OOH+R30C8H17    1.8E+0013  0.000  20000.0  ! ME 157
CN
C8H18-1+R8CH3OO=>CH3OOH+R31C8H17    1.2E+0013  0.000  20000.0  ! ME 158
CN
C8H18-1+R8CH3OO=>CH3OOH+R32C8H17    1.5E+0012  0.000  15000.0  ! ME 159
CN
C8H18-1+R8CH3OO=>CH3OOH+R33C8H17    3.0E+0012  0.000  17500.0  ! ME 160
CN
C7H16-1+R11C2H5=>C2H6+R26C7H15    2.0E+0011  0.000  11000.0  ! ME 161 CN
C7H16-1+R11C2H5=>C2H6+R27C7H15    6.0E+0011  0.000  13500.0  ! ME 162 CR
C7H16-1+R11C2H5=>C2H6+R28C7H15    4.0E+0011  0.000  11000.0  ! ME 163 CN
C7H16-1+R11C2H5=>C2H6+R29C7H15    4.0E+0011  0.000  11000.0  ! ME 164 CN
C8H18-1+R11C2H5=>C2H6+R30C8H17    9.0E+0011  0.000  13500.0  ! ME 165 CR
C8H18-1+R11C2H5=>C2H6+R31C8H17    6.0E+0011  0.000  13500.0  ! ME 166 CR
C8H18-1+R11C2H5=>C2H6+R32C8H17    1.0E+0011  0.000  9200.0  ! ME 167 CN
C8H18-1+R11C2H5=>C2H6+R33C8H17    2.0E+0011  0.000  11000.0  ! ME 168 CN
C7H16-1+R38C4H9=>C4H10+R26C7H15    1.0E+0011  0.000  12700.0  ! ME 169 CR
C7H16-1+R38C4H9=>C4H10+R27C7H15    3.0E+0011  0.000  15000.0  ! ME 170 CR
C7H16-1+R38C4H9=>C4H10+R28C7H15    2.0E+0011  0.000  12700.0  ! ME 171 CR
C7H16-1+R38C4H9=>C4H10+R29C7H15    2.0E+0011  0.000  12700.0  ! ME 172 CR
C8H18-1+R38C4H9=>C4H10+R30C8H17    4.5E+0011  0.000  15000.0  ! ME 173 CR
C8H18-1+R38C4H9=>C4H10+R31C8H17    3.0E+0011  0.000  15000.0  ! ME 174 CR
C8H18-1+R38C4H9=>C4H10+R32C8H17    5.0E+0010  0.000  11100.0  ! ME 175 CR
C8H18-1+R38C4H9=>C4H10+R33C8H17    1.0E+0011  0.000  12700.0  ! ME 176 CR

!   combinations :
R1H+R38C4H9=>C4H10    8.3E+0012  0.000  0.0  ! CO 177 KB
R1H+R43C3H7=>C3H8    8.3E+0012  0.000  0.0  ! CO 178 KB
R2OH+R38C4H9=>C4H10OL    5.7E+0012  0.000  0.0  ! CO 179 KB
R2OH+R43C3H7=>C3H7OH    5.9E+0012  0.000  0.0  ! CO 180 KB
R3OOH+R38C4H9=>C4H10O2P    4.5E+0012  0.000  0.0  ! CO 181 KB
R3OOH+R43C3H7=>C3H8O2P    4.8E+0012  0.000  0.0  ! CO 182 KB
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R4CH3+R38C4H9=>C5H12    1.5E+0013  0.000  0.0  ! CO 183 KB
R4CH3+R43C3H7=>C4H10    1.5E+0013  0.000  0.0  ! CO 184 KB
R5CHO+R38C4H9=>C5H10OA    4.9E+0012  0.000  0.0  ! CO 185 KB
R5CHO+R43C3H7=>C4H8OA    5.2E+0012  0.000  0.0  ! CO 186 KB
R6CH2OH+R38C4H9=>C5H12OL    4.8E+0012  0.000  0.0  ! CO 187 KB
R6CH2OH+R43C3H7=>C4H10OL    5.1E+0012  0.000  0.0  ! CO 188 KB
R11C2H5+R38C4H9=>C6H14    4.9E+0012  0.000  0.0  ! CO 189 KB
R11C2H5+R43C3H7=>C5H12    5.2E+0012  0.000  0.0  ! CO 190 KB
R38C4H9+R38C4H9=>C8H18    2.0E+0012  0.000  0.0  ! CO 191 KB
R38C4H9+R43C3H7=>C7H16    4.3E+0012  0.000  0.0  ! CO 192 KB
R43C3H7+R43C3H7=>C6H14    2.3E+0012  0.000  0.0  ! CO 193 KB

!   dismutations :

!    -------------------
!    SECONDARY MECHANISM
!    -------------------

!    Peroxide decomposition

! Hydroperoxide decomposition
C4H10O2P=>R2OH+R11C2H5+CH3CHO    1.5E+0016  0.000  43000.0  ! DHP 194
C3H8O2P=>R2OH+R11C2H5+HCHO    1.5E+0016  0.000  43000.0  ! DHP 195
C3H6O2PY=>R2OH+R1H+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 196
C4H8O2PY=>R2OH+R4CH3+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 197
C7H14O2PY=>R2OH+R20C4H9+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 198
C8H16O2PY=>R2OH+R35C5H11+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 199
C5H10O2PY=>R2OH+R11C2H5+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions
C3H8+R1H=>H2+R19C3H7    5.7E+0007  2.000  7700.0  ! MH 201
     DUPLICATE
C3H8+R1H=>H2+R19C3H7    9.0E+0006  2.000  5000.0  ! MH 202
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    5.4E+0006  2.000  450.0  ! MH 203
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    2.6E+0006  2.000  -765.0  ! MH 204
     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    1.2E+0012  0.000  17000.0  ! MH 205
     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    4.0E+0011  0.000  15500.0  ! MH 206
     DUPLICATE
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C3H8+R4CH3=>CH4+R19C3H7    6.0E-0001  4.000  8200.0  ! MH 207
     DUPLICATE
C3H8+R4CH3=>CH4+R19C3H7    2.0E+0011  0.000  9600.0  ! MH 208
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    1.2E+0013  0.000  20000.0  ! MH 209
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    3.0E+0012  0.000  17500.0  ! MH 210
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! MH 211
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    2.0E+0011  0.000  11000.0  ! MH 212
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    5.7E+0007  2.000  7700.0  ! MH 213
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    1.8E+0007  2.000  5000.0  ! MH 214
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.4E+0006  2.000  450.0  ! MH 215
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.2E+0006  2.000  -765.0  ! MH 216
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    1.2E+0012  0.000  17000.0  ! MH 217
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    8.0E+0011  0.000  15500.0  ! MH 218
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    6.0E-0001  4.000  8200.0  ! MH 219
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    4.0E+0011  0.000  9600.0  ! MH 220
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    1.2E+0013  0.000  20000.0  ! MH 221
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    6.0E+0012  0.000  17500.0  ! MH 222
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    6.0E+0011  0.000  13500.0  ! MH 223
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    4.0E+0011  0.000  11000.0  ! MH 224
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    5.7E+0007  2.000  7700.0  ! MH 225
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    2.7E+0007  2.000  5000.0  ! MH 226
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    5.4E+0006  2.000  450.0  ! MH 227
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    7.8E+0006  2.000  -765.0  ! MH 228
     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  17000.0  ! MH 229
     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  15500.0  ! MH 230
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E-0001  4.000  8200.0  ! MH 231
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E+0011  0.000  9600.0  ! MH 232
     DUPLICATE
C5H12+R8CH3OO=>CH3OOH+R35C5H11    1.2E+0013  0.000  20000.0  ! MH 233
     DUPLICATE
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C5H12+R8CH3OO=>CH3OOH+R35C5H11    9.0E+0012  0.000  17500.0  ! MH 234
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  13500.0  ! MH 235
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  11000.0  ! MH 236
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    5.7E+0007  2.000  7700.0  ! MH 237
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    3.6E+0007  2.000  5000.0  ! MH 238
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    5.4E+0006  2.000  450.0  ! MH 239
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    1.0E+0007  2.000  -765.0  ! MH 240
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.2E+0012  0.000  17000.0  ! MH 241
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.6E+0012  0.000  15500.0  ! MH 242
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    6.0E-0001  4.000  8200.0  ! MH 243
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    8.0E+0011  0.000  9600.0  ! MH 244
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  20000.0  ! MH 245
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  17500.0  ! MH 246
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    6.0E+0011  0.000  13500.0  ! MH 247
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    8.0E+0011  0.000  11000.0  ! MH 248
     DUPLICATE

! O-ring decomposition
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 249
     DUPLICATE
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    1.3E+0007  2.000  5000.0  ! DE# 250
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 251
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    3.9E+0006  2.000  -765.0  ! DE# 252
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  17000.0  ! DE# 253
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  15500.0  ! DE# 254
     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 255
     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E+0011  0.000  9600.0  ! DE# 256
     DUPLICATE
C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    6.0E+0012  0.000  20000.0  ! DE#
257
     DUPLICATE
C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    4.5E+0012  0.000  17500.0  ! DE#
258
     DUPLICATE
```

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C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
259
     DUPLICATE
C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  11000.0  ! DE#
260
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 261
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.3E+0007  2.000  5000.0  ! DE# 262
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 263
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    6.5E+0006  2.000  -765.0  ! DE# 264
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
265
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    1.0E+0012  0.000  15500.0  ! DE#
266
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 267
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    5.0E+0011  0.000  9600.0  ! DE# 268
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 269
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    7.5E+0012  0.000  17500.0  !
DE# 270
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
271
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    5.0E+0011  0.000  11000.0  ! DE#
272
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 273
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    3.2E+0007  2.000  5000.0  ! DE# 274
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 275
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    9.1E+0006  2.000  -765.0  ! DE# 276
     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
277
     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    1.4E+0012  0.000  15500.0  ! DE#
278
     DUPLICATE
C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    3.0E-0001  4.000  8200.0  ! DE#
279
     DUPLICATE
```

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C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    7.0E+0011  0.000  9600.0  ! DE#
280
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 281
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    1.0E+0013  0.000  17500.0  !
DE# 282
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    3.0E+0011  0.000  13500.0  !
DE# 283
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    7.0E+0011  0.000  11000.0  !
DE# 284
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 285
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    5.0E+0007  2.000  5000.0  ! DE# 286
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
287
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    1.4E+0007  2.000  -765.0  ! DE#
288
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 289
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    2.2E+0012  0.000  15500.0  !
DE# 290
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
291
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  9600.0  ! DE#
292
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 293
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    1.7E+0013  0.000
17500.0  ! DE# 294
     DUPLICATE
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 295
     DUPLICATE
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  11000.0  !
DE# 296
     DUPLICATE
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 297
     DUPLICATE
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    4.1E+0007  2.000  5000.0  ! DE# 298
     DUPLICATE
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C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
299
     DUPLICATE
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    1.1E+0007  2.000  -765.0  ! DE#
300
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 301
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    1.8E+0012  0.000  15500.0  !
DE# 302
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
303
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  9600.0  ! DE#
304
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 305
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    1.3E+0013  0.000
17500.0  ! DE# 306
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 307
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  11000.0  !
DE# 308
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE# 309
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    5.9E+0007  2.000  5000.0  ! DE# 310
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE# 311
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    1.7E+0007  2.000  -765.0  ! DE#
312
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    6.0E+0011  0.000  17000.0  ! DE#
313
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    2.6E+0012  0.000  15500.0  ! DE#
314
     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
315
     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    1.3E+0012  0.000  9600.0  ! DE#
316
     DUPLICATE
C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    6.0E+0012  0.000  20000.0  !
DE# 317
     DUPLICATE
```

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C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    2.0E+0013  0.000  17500.0  !
DE# 318
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 319
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    1.3E+0012  0.000  11000.0  !
DE# 320
     DUPLICATE
C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE# 321
     DUPLICATE
C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    6.8E+0007  2.000  5000.0  ! DE# 322
     DUPLICATE
C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE#
323
     DUPLICATE
C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.0E+0007  2.000  -765.0  ! DE#
324
     DUPLICATE
C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    6.0E+0011  0.000  17000.0  !
DE# 325
     DUPLICATE
C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    3.0E+0012  0.000  15500.0  !
DE# 326
     DUPLICATE
C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
327
     DUPLICATE
C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    1.5E+0012  0.000  9600.0  ! DE#
328
     DUPLICATE
C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    6.0E+0012  0.000
20000.0  ! DE# 329
     DUPLICATE
C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    2.3E+0013  0.000
17500.0  ! DE# 330
     DUPLICATE
C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 331
     DUPLICATE
C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    1.5E+0012  0.000  11000.0  !
DE# 332
     DUPLICATE
C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
333
     DUPLICATE
C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    7.7E+0007  2.000  5000.0  ! DE#
334
     DUPLICATE
C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
335
     DUPLICATE
C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.2E+0007  2.000  -765.0  ! DE#
336
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     DUPLICATE
C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 337
     DUPLICATE
C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    3.4E+0012  0.000  15500.0  !
DE# 338
     DUPLICATE
C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    3.0E-0001  4.000  8200.0  ! DE#
339
     DUPLICATE
C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    1.7E+0012  0.000  9600.0  ! DE#
340
     DUPLICATE
C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 341
     DUPLICATE
C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    2.6E+0013  0.000  17500.0
! DE# 342
     DUPLICATE
C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    3.0E+0011  0.000  13500.0  !
DE# 343
     DUPLICATE
C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    1.7E+0012  0.000  11000.0  !
DE# 344
     DUPLICATE
C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
345
     DUPLICATE
C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    1.0E+0008  2.000  5000.0  ! DE#
346
     DUPLICATE
C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
347
     DUPLICATE
C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    3.0E+0007  2.000  -765.0  ! DE#
348
     DUPLICATE
C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 349
     DUPLICATE
C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    4.6E+0012  0.000  15500.0  !
DE# 350
     DUPLICATE
C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 351
     DUPLICATE
C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    2.3E+0012  0.000  9600.0  !
DE# 352
     DUPLICATE
C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    6.0E+0012  0.000  20000.0
! DE# 353
     DUPLICATE
C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    3.5E+0013  0.000  17500.0
! DE# 354
```

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     DUPLICATE
C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    3.0E+0011  0.000
13500.0  ! DE# 355
     DUPLICATE
C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    2.3E+0012  0.000
11000.0  ! DE# 356
     DUPLICATE
C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
357
     DUPLICATE
C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    9.5E+0007  2.000  5000.0  ! DE#
358
     DUPLICATE
C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
359
     DUPLICATE
C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0007  2.000  -765.0  ! DE#
360
     DUPLICATE
C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 361
     DUPLICATE
C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    4.2E+0012  0.000  15500.0  !
DE# 362
     DUPLICATE
C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 363
     DUPLICATE
C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    2.1E+0012  0.000  9600.0  !
DE# 364
     DUPLICATE
C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    6.0E+0012  0.000  20000.0
! DE# 365
     DUPLICATE
C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    3.2E+0013  0.000  17500.0
! DE# 366
     DUPLICATE
C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    3.0E+0011  0.000
13500.0  ! DE# 367
     DUPLICATE
C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    2.1E+0012  0.000
11000.0  ! DE# 368
     DUPLICATE
C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
369
     DUPLICATE
C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    8.6E+0007  2.000  5000.0  ! DE#
370
     DUPLICATE
C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
371
     DUPLICATE
C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.5E+0007  2.000  -765.0  ! DE#
372
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     DUPLICATE
C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 373
     DUPLICATE
C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    3.8E+0012  0.000  15500.0  !
DE# 374
     DUPLICATE
C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    3.0E-0001  4.000  8200.0  ! DE#
375
     DUPLICATE
C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    1.9E+0012  0.000  9600.0  ! DE#
376
     DUPLICATE
C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 377
     DUPLICATE
C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    2.9E+0013  0.000  17500.0
! DE# 378
     DUPLICATE
C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    3.0E+0011  0.000  13500.0  !
DE# 379
     DUPLICATE
C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    1.9E+0012  0.000  11000.0  !
DE# 380
     DUPLICATE
C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    2.9E+0007  2.000  7700.0  ! DE#
381
     DUPLICATE
C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    1.1E+0008  2.000  5000.0  ! DE#
382
     DUPLICATE
C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    2.7E+0006  2.000  450.0  ! DE#
383
     DUPLICATE
C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    3.3E+0007  2.000  -765.0  ! DE#
384
     DUPLICATE
C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    6.0E+0011  0.000  17000.0  !
DE# 385
     DUPLICATE
C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    5.0E+0012  0.000  15500.0  !
DE# 386
     DUPLICATE
C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    3.0E-0001  4.000  8200.0  !
DE# 387
     DUPLICATE
C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    2.5E+0012  0.000  9600.0  !
DE# 388
     DUPLICATE
C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    6.0E+0012  0.000  20000.0
! DE# 389
     DUPLICATE
C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    3.8E+0013  0.000  17500.0
! DE# 390
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     DUPLICATE
C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    3.0E+0011  0.000
13500.0  ! DE# 391
     DUPLICATE
C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    2.5E+0012  0.000
11000.0  ! DE# 392
     DUPLICATE


! Metatheses of oxetanes, furanes and pyranes

! decompositions of cyclo-ether radicals

! Addition of oxygen on cyclo-ether radicals
!    O2 elimination
!    Isomerization
!    Cylo-ether keto-hydroperoxide ester formation
!    Decomposition of cylo-ether keto-hydroperoxide ester

! Isomerization of peroxy-radicals

!Addition of oxygen on cyclo-peroxy radicals

! Formation of cyclo-ether ketohydroperoxydes

! Decomposition of cyclo-ether ketohydroperoxydes

! Olefin reactions
!  addition of H and CH3 on olefins
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  1560.0  ! ADZ 393
     DUPLICATE
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  3260.0  ! ADZ 394
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  1560.0  ! ADZ 395
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  3260.0  ! ADZ 396
     DUPLICATE
C4H8Y+R4CH3=>C3H6Y+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 397
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 398
     DUPLICATE
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 399
     DUPLICATE
C5H10Z+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 400
C5H10Z+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 401
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 402
     DUPLICATE
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 403
     DUPLICATE
C7H14Z+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 404
C7H14Z+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 405
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  1560.0  ! ADZ 406
     DUPLICATE
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  3260.0  ! ADZ 407
     DUPLICATE
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C6H12Z+R4CH3=>C4H8Y+R19C3H7    1.7E+0011  0.000  7400.0  ! ADZ 408
C6H12Z+R4CH3=>C3H6Y+R20C4H9    9.6E+0010  0.000  8000.0  ! ADZ 409
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 410
     DUPLICATE
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 411
     DUPLICATE
C7H14Y+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 412
C7H14Y+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 413
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 414
     DUPLICATE
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 415
     DUPLICATE
C8H16Y+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 416
C8H16Y+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 417
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 418
     DUPLICATE
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 419
     DUPLICATE
C8H16Z+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 420
C8H16Z+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 421
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 422
     DUPLICATE
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 423
     DUPLICATE
C5H10Y+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 424
C5H10Y+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 425
C9H18Z+R4CH3=>C4H8Y+R41C6H13    1.7E+0011  0.000  7400.0  ! ADZ 426
C9H18Z+R4CH3=>C3H6Y+R26C7H15    9.6E+0010  0.000  8000.0  ! ADZ 427
C10H20Z+R4CH3=>C4H8Y+R26C7H15    1.7E+0011  0.000  7400.0  ! ADZ 428
C10H20Z+R4CH3=>C3H6Y+R30C8H17    9.6E+0010  0.000  8000.0  ! ADZ 429
C11H22Z+R4CH3=>C4H8Y+R30C8H17    1.7E+0011  0.000  7400.0  ! ADZ 430
C9H18Z+R1H=>4C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 431
C10H20Z+R1H=>4C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 432
C13H26Z+R1H=>6C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 433
C12H24Z+R1H=>5C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 434
C11H22Z+R1H=>5C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 435
C14H28Z+R1H=>6C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 436

!  addition of OH on olefins
C3H6Y+R2OH=>R4CH3+CH3CHO    1.4E+0012  0.000  -1040.0  ! ADZ 437
C3H6Y+R2OH=>R11C2H5+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 438
C4H8Y+R2OH=>R4CH3+C2H5CHO    1.4E+0012  0.000  -1040.0  ! ADZ 439
C4H8Y+R2OH=>R19C3H7+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 440
C5H10Z+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 441
C5H10Z+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 442
C7H14Z+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 443
C7H14Z+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 444
C6H12Z+R2OH=>R4CH3+C5H10OA    1.4E+0012  0.000  -1040.0  ! ADZ 445
C6H12Z+R2OH=>R35C5H11+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 446
C7H14Y+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 447
C7H14Y+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 448
C8H16Y+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 449
C8H16Y+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 450
C8H16Z+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 451
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C8H16Z+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 452
C5H10Y+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 453
C5H10Y+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 454
C9H18Z+R2OH=>R4CH3+C8H16OA    1.4E+0012  0.000  -1040.0  ! ADZ 455
C9H18Z+R2OH=>R30C8H17+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 456
C10H20Z+R2OH=>R4CH3+C9H18OA    1.4E+0012  0.000  -1040.0  ! ADZ 457
C13H26Z+R2OH=>R4CH3+C12H24OA    1.4E+0012  0.000  -1040.0  ! ADZ 458
C12H24Z+R2OH=>R4CH3+C11H22OA    1.4E+0012  0.000  -1040.0  ! ADZ 459
C11H22Z+R2OH=>R4CH3+C10H20OA    1.4E+0012  0.000  -1040.0  ! ADZ 460
C14H28Z+R2OH=>R4CH3+C13H26OA    1.4E+0012  0.000  -1040.0  ! ADZ 461

C10H20Z+R2OH=>HCHO+R4CH3+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 462
C13H26Z+R2OH=>HCHO+R11C2H5+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 463
C12H24Z+R2OH=>HCHO+R4CH3+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 464
C11H22Z+R2OH=>HCHO+R11C2H5+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 465
C14H28Z+R2OH=>HCHO+R4CH3+6C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 466

!  addition of O on olefins
C3H6Y+B1O=>CH2COZ+R1H+R4CH3    1.2E+0005  2.560  -1130.0  ! AOZ 467
C4H8Y+B1O=>CH2COZ+R1H+R11C2H5    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Z+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Z+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C6H12Z+B1O=>CH2COZ+R1H+R20C4H9    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Y+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Y+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Z+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Y+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
C9H18Z+B1O=>CH2COZ+R1H+R26C7H15    1.2E+0005  2.560  -1130.0  ! AOZ 467
C10H20Z+B1O=>CH2COZ+R1H+R30C8H17    1.2E+0005  2.560  -1130.0  ! AOZ 467
!C13H26Z+B1O=>CH2COZ+R4CH3+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C12H24Z+B1O=>CH2COZ+R11C2H5+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467
!C11H22Z+B1O=>CH2COZ+R4CH3+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C14H28Z+B1O=>CH2COZ+R11C2H5+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467

! retroene reactions
C5H10Z=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 467
C7H14Z=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 468
C6H12Z=>C3H6Y+C3H6Y    8.0E+0012  0.000  56500.0  ! RTZ 469
C7H14Y=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 470
C8H16Y=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 471
C8H16Z=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 472
C5H10Y=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 473
C9H18Z=>C3H6Y+C6H12Z    8.0E+0012  0.000  56500.0  ! RTZ 474
C10H20Z=>C3H6Y+C7H14Z    8.0E+0012  0.000  56500.0  ! RTZ 475
C13H26Z=>C3H6Y+C10H20Z    8.0E+0012  0.000  56500.0  ! RTZ 476
C12H24Z=>C3H6Y+C9H18Z    8.0E+0012  0.000  56500.0  ! RTZ 477
C11H22Z=>C3H6Y+C8H16Z    8.0E+0012  0.000  56500.0  ! RTZ 478
C14H28Z=>C3H6Y+C11H22Z    8.0E+0012  0.000  56500.0  ! RTZ 479

!  addition of OOH on olefins
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C3H6Y+R3OOH=>R2OH+C3H6OE#3    1.0E+0012  0.000  14200.0  ! ADZ 480
C4H8Y+R3OOH=>R2OH+C4H8OE#3    1.0E+0012  0.000  14200.0  ! ADZ 481
C5H10Z+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 482
C7H14Z+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 483
C6H12Z+R3OOH=>R2OH+C6H12OE#3    1.0E+0012  0.000  14200.0  ! ADZ 484
C7H14Y+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 485
C8H16Y+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 486
C8H16Z+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 487
C5H10Y+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 488
C9H18Z+R3OOH=>R2OH+C9H18OE#3    1.0E+0012  0.000  14200.0  ! ADZ 489
C10H20Z+R3OOH=>R2OH+C10H20OE#3    1.0E+0012  0.000  14200.0  ! ADZ 490
C13H26Z+R3OOH=>R2OH+C13H26OE#3    1.0E+0012  0.000  14200.0  ! ADZ 491
C12H24Z+R3OOH=>R2OH+C12H24OE#3    1.0E+0012  0.000  14200.0  ! ADZ 492
C11H22Z+R3OOH=>R2OH+C11H22OE#3    1.0E+0012  0.000  14200.0  ! ADZ 493
C14H28Z+R3OOH=>R2OH+C14H28OE#3    1.0E+0012  0.000  14200.0  ! ADZ 494

!   olefin to dienes
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    5.4E+0004  2.500  -1900.0  ! MZ 495
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    2.9E+0007  2.000  7700.0  ! MZ 496
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    9.0E+0006  2.000  5000.0  ! MZ 497
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    3.0E+0006  2.000  -1520.0  ! MZ 498
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.7E+0006  2.000  450.0  ! MZ 499
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.6E+0006  2.000  -765.0  ! MZ 500
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.4E+0003  2.600  12400.0  ! MZ 501
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.0E+0011  0.000  17000.0  ! MZ 502
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    4.0E+0011  0.000  15500.0  ! MZ 503
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    1.0E+0011  0.000  7300.0  ! MZ 504
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    3.0E-0001  4.000  8200.0  ! MZ 505
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    2.0E+0011  0.000  9600.0  ! MZ 506
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    1.0E+0012  0.000  14550.0  ! MZ
507
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    6.0E+0012  0.000  20000.0  ! MZ
508
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    3.0E+0012  0.000  17500.0  ! MZ
509
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    1.5E+0000  3.500  4140.0  ! MZ 510
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    3.0E+0011  0.000  13500.0  ! MZ 511
     DUPLICATE
```

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C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    2.0E+0011  0.000  11000.0  ! MZ 512
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    5.4E+0004  2.500  -1900.0  ! MZ 513
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.9E+0007  2.000  7700.0  ! MZ 514
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.7E+0007  2.000  5000.0  ! MZ 515
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    3.0E+0006  2.000  -1520.0  ! MZ 516
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    2.7E+0006  2.000  450.0  ! MZ 517
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    7.8E+0006  2.000  -765.0  ! MZ 518
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.4E+0003  2.600  12400.0  ! MZ 519
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.0E+0011  0.000  17000.0  ! MZ 520
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    1.2E+0012  0.000  15500.0  ! MZ 521
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    1.0E+0011  0.000  7300.0  ! MZ 522
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    3.0E-0001  4.000  8200.0  ! MZ 523
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    6.0E+0011  0.000  9600.0  ! MZ 524
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    1.0E+0012  0.000  14550.0  ! MZ
525
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    6.0E+0012  0.000  20000.0  ! MZ
526
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    9.0E+0012  0.000  17500.0  ! MZ
527
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    1.5E+0000  3.500  4140.0  ! MZ 528
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    3.0E+0011  0.000  13500.0  ! MZ
529
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    6.0E+0011  0.000  11000.0  ! MZ
530
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    5.4E+0004  2.500  -1900.0  ! MZ 531
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    2.9E+0007  2.000  7700.0  ! MZ 532
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    1.8E+0007  2.000  5000.0  ! MZ 533
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    3.0E+0006  2.000  -1520.0  ! MZ 534
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    2.7E+0006  2.000  450.0  ! MZ 535
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    5.2E+0006  2.000  -765.0  ! MZ 536
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     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.4E+0003  2.600  12400.0  ! MZ 537
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.0E+0011  0.000  17000.0  ! MZ 538
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    8.0E+0011  0.000  15500.0  ! MZ 539
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    1.0E+0011  0.000  7300.0  ! MZ 540
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    3.0E-0001  4.000  8200.0  ! MZ 541
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    4.0E+0011  0.000  9600.0  ! MZ 542
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    1.0E+0012  0.000  14550.0  ! MZ
543
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  20000.0  ! MZ
544
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  17500.0  ! MZ
545
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    1.5E+0000  3.500  4140.0  ! MZ 546
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    3.0E+0011  0.000  13500.0  ! MZ
547
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    4.0E+0011  0.000  11000.0  ! MZ
548
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    5.4E+0004  2.500  -1900.0  ! MZ 549
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    2.9E+0007  2.000  7700.0  ! MZ 550
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    3.6E+0007  2.000  5000.0  ! MZ 551
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    3.0E+0006  2.000  -1520.0  ! MZ 552
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    2.7E+0006  2.000  450.0  ! MZ 553
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    1.0E+0007  2.000  -765.0  ! MZ 554
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.4E+0003  2.600  12400.0  ! MZ 555
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.0E+0011  0.000  17000.0  ! MZ 556
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    1.6E+0012  0.000  15500.0  ! MZ 557
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    1.0E+0011  0.000  7300.0  ! MZ 558
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    3.0E-0001  4.000  8200.0  ! MZ 559
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    8.0E+0011  0.000  9600.0  ! MZ 560
     DUPLICATE
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C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.0E+0012  0.000  14550.0  ! MZ
561
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    6.0E+0012  0.000  20000.0  ! MZ
562
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.2E+0013  0.000  17500.0  ! MZ
563
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    1.5E+0000  3.500  4140.0  ! MZ 564
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    3.0E+0011  0.000  13500.0  ! MZ
565
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    8.0E+0011  0.000  11000.0  ! MZ
566
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    5.4E+0004  2.500  -1900.0  ! MZ 567
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    2.9E+0007  2.000  7700.0  ! MZ 568
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    4.5E+0007  2.000  5000.0  ! MZ 569
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    3.0E+0006  2.000  -1520.0  ! MZ 570
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    2.7E+0006  2.000  450.0  ! MZ 571
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    1.3E+0007  2.000  -765.0  ! MZ 572
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.4E+0003  2.600  12400.0  ! MZ 573
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.0E+0011  0.000  17000.0  ! MZ 574
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    2.0E+0012  0.000  15500.0  ! MZ 575
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0011  0.000  7300.0  ! MZ 576
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    3.0E-0001  4.000  8200.0  ! MZ 577
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0012  0.000  9600.0  ! MZ 578
     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.0E+0012  0.000  14550.0  ! MZ
579
     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    6.0E+0012  0.000  20000.0  ! MZ
580
     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.5E+0013  0.000  17500.0  ! MZ
581
     DUPLICATE
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.5E+0000  3.500  4140.0  ! MZ
582
     DUPLICATE
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C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    3.0E+0011  0.000  13500.0  ! MZ
583
     DUPLICATE
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.0E+0012  0.000  11000.0  ! MZ
584
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0004  2.500  -1900.0  ! MZ 585
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    2.9E+0007  2.000  7700.0  ! MZ 586
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0007  2.000  5000.0  ! MZ 587
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    3.0E+0006  2.000  -1520.0  ! MZ 588
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    2.7E+0006  2.000  450.0  ! MZ 589
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    1.5E+0007  2.000  -765.0  ! MZ 590
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.4E+0003  2.600  12400.0  ! MZ
591
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.0E+0011  0.000  17000.0  ! MZ
592
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    2.4E+0012  0.000  15500.0  ! MZ
593
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.0E+0011  0.000  7300.0  ! MZ 594
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    3.0E-0001  4.000  8200.0  ! MZ 595
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.2E+0012  0.000  9600.0  ! MZ 596
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.0E+0012  0.000  14550.0  !
MZ 597
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    6.0E+0012  0.000  20000.0  !
MZ 598
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.8E+0013  0.000  17500.0  !
MZ 599
     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.5E+0000  3.500  4140.0  ! MZ
600
     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    3.0E+0011  0.000  13500.0  ! MZ
601
     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.2E+0012  0.000  11000.0  ! MZ
602
     DUPLICATE
!C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
603
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!C13H26Z+R2OH=>H2O+C4H6Z2+R4CH3+4C2H4Z    3.0E+0006  2.000  -1520.0  ! MZ
604
!C13H26Z+R3OOH=>H2O2+C4H6Z2+R4CH3+4C2H4Z    6.4E+0003  2.600  12400.0  !
MZ 605
!C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0  ! MZ
606
!C13H26Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0
! MZ 607
!C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z    1.5E+0000  3.500  4140.0  !
MZ 608
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    5.4E+0004  2.500  -1900.0  ! MZ 609
     DUPLICATE
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    2.9E+0007  2.000  7700.0  ! MZ 610
     DUPLICATE
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    7.2E+0007  2.000  5000.0  ! MZ 611
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    3.0E+0006  2.000  -1520.0  ! MZ 612
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.7E+0006  2.000  450.0  ! MZ 613
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.1E+0007  2.000  -765.0  ! MZ 614
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.4E+0003  2.600  12400.0  ! MZ
615
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.0E+0011  0.000  17000.0  ! MZ
616
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    3.2E+0012  0.000  15500.0  ! MZ
617
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.0E+0011  0.000  7300.0  ! MZ 618
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    3.0E-0001  4.000  8200.0  ! MZ 619
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.6E+0012  0.000  9600.0  ! MZ 620
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    1.0E+0012  0.000  14550.0  !
MZ 621
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    6.0E+0012  0.000  20000.0  !
MZ 622
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    2.4E+0013  0.000  17500.0  !
MZ 623
     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.5E+0000  3.500  4140.0  ! MZ
624
     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    3.0E+0011  0.000  13500.0  ! MZ
625
     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.6E+0012  0.000  11000.0  ! MZ
626
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     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    5.4E+0004  2.500  -1900.0  ! MZ 627
     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    2.9E+0007  2.000  7700.0  ! MZ 628
     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    6.3E+0007  2.000  5000.0  ! MZ 629
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    3.0E+0006  2.000  -1520.0  ! MZ 630
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    2.7E+0006  2.000  450.0  ! MZ 631
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    1.8E+0007  2.000  -765.0  ! MZ 632
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.4E+0003  2.600  12400.0  ! MZ
633
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.0E+0011  0.000  17000.0  ! MZ
634
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    2.8E+0012  0.000  15500.0  ! MZ
635
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.0E+0011  0.000  7300.0  ! MZ 636
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    3.0E-0001  4.000  8200.0  ! MZ 637
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.4E+0012  0.000  9600.0  ! MZ 638
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    1.0E+0012  0.000  14550.0  !
MZ 639
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    6.0E+0012  0.000  20000.0  !
MZ 640
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    2.1E+0013  0.000  17500.0  !
MZ 641
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.5E+0000  3.500  4140.0  ! MZ
642
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    3.0E+0011  0.000  13500.0  ! MZ
643
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.4E+0012  0.000  11000.0  ! MZ
644
     DUPLICATE
!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
645
!C14H28Z+R2OH=>H2O+C4H6Z2+R11C2H5+4C2H4Z    3.0E+0006  2.000  -1520.0  !
MZ 646
!C14H28Z+R3OOH=>H2O2+C4H6Z2+R11C2H5+4C2H4Z    6.4E+0003  2.600
12400.0  ! MZ 647
!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000  7300.0  !
MZ 648
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!C14H28Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000
7300.0  ! MZ 649
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z    1.5E+0000  3.500  4140.0
! MZ 650
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    8.8E+0010  0.700  3250.0  ! MZ 651
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    5.1E+0013  0.000  7850.0  ! MZ 652
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    2.6E+0013  0.000  5200.0  ! MZ 653
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    8.8E+0010  0.700  3250.0  ! MZ 654
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    5.1E+0013  0.000  7850.0  ! MZ 655
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    7.8E+0013  0.000  5200.0  ! MZ 656
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    8.8E+0010  0.700  3250.0  ! MZ 657
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.1E+0013  0.000  7850.0  ! MZ 658
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.2E+0013  0.000  5200.0  ! MZ 659
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    8.8E+0010  0.700  3250.0  ! MZ 660
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    5.1E+0013  0.000  7850.0  ! MZ 661
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    1.0E+0014  0.000  5200.0  ! MZ 662
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    8.8E+0010  0.700  3250.0  ! MZ 663
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    5.1E+0013  0.000  7850.0  ! MZ 664
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    1.3E+0014  0.000  5200.0  ! MZ 665
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    8.8E+0010  0.700  3250.0  ! MZ 666
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    5.1E+0013  0.000  7850.0  ! MZ 667
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    1.6E+0014  0.000  5200.0  ! MZ 668
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    8.8E+0010  0.700  3250.0  ! MZ 669
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    5.1E+0013  0.000  7850.0  ! MZ 670
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    2.1E+0014  0.000  5200.0  ! MZ 671
     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    8.8E+0010  0.700  3250.0  ! MZ 672
     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    5.1E+0013  0.000  7850.0  ! MZ 673
     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    1.8E+0014  0.000  5200.0  ! MZ 674
     DUPLICATE

! Metathesis with YH
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C3H6Y+R1H=>RC3H5Y+H2    1.7E+0005  2.500  2510.0  ! MES 675
C3H6Y+R2OH=>RC3H5Y+H2O    3.0E+0006  2.000  -298.0  ! MES 676
C3H6Y+R3OOH=>RC3H5Y+H2O2    9.6E+0003  2.600  13900.0  ! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4    2.2E+0000  3.500  5670.0  ! MES 678
C3H6Y+R8CH3OO=>RC3H5Y+CH3OOH    2.0E+0012  0.000  17050.0  ! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6    2.2E+0000  3.500  6640.0  ! MES 680
C4H8Y+R1H=>RC4H7Y+H2    5.4E+0004  2.500  -1900.0  ! MES 681
     DUPLICATE
C4H8Y+R1H=>RC4H7Y+H2    2.9E+0007  2.000  7700.0  ! MES 682
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 683
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    2.7E+0006  2.000  450.0  ! MES 684
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 685
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 686
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    1.0E+0011  0.000  7300.0  ! MES 687
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    3.0E-0001  4.000  8200.0  ! MES 688
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 689
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 690
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 691
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 692
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    5.4E+0004  2.500  -1900.0  ! MES 693
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.9E+0007  2.000  7700.0  ! MES 694
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.7E+0007  2.000  5000.0  ! MES 695
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 696
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    2.7E+0006  2.000  450.0  ! MES 697
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    7.8E+0006  2.000  -765.0  ! MES 698
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 699
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 700
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    1.2E+0012  0.000  15500.0  ! MES 701
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    1.0E+0011  0.000  7300.0  ! MES 702
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    3.0E-0001  4.000  8200.0  ! MES 703
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    6.0E+0011  0.000  9600.0  ! MES 704
     DUPLICATE
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C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 705
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 706
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    9.0E+0012  0.000  17500.0  ! MES 707
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 708
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 709
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    6.0E+0011  0.000  11000.0  ! MES 710
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    5.4E+0004  2.500  -1900.0  ! MES 711
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    2.9E+0007  2.000  7700.0  ! MES 712
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    3.6E+0007  2.000  5000.0  ! MES 713
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 714
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    2.7E+0006  2.000  450.0  ! MES 715
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    1.0E+0007  2.000  -765.0  ! MES 716
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 717
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 718
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    1.6E+0012  0.000  15500.0  ! MES 719
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    1.0E+0011  0.000  7300.0  ! MES 720
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    3.0E-0001  4.000  8200.0  ! MES 721
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    8.0E+0011  0.000  9600.0  ! MES 722
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 723
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 724
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.2E+0013  0.000  17500.0  ! MES 725
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 726
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 727
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    8.0E+0011  0.000  11000.0  ! MES 728
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    5.4E+0004  2.500  -1900.0  ! MES 729
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    2.9E+0007  2.000  7700.0  ! MES 730
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    9.0E+0006  2.000  5000.0  ! MES 731
     DUPLICATE
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C5H10Y+R2OH=>RC5H9Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 732
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.7E+0006  2.000  450.0  ! MES 733
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.6E+0006  2.000  -765.0  ! MES 734
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 735
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 736
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    4.0E+0011  0.000  15500.0  ! MES 737
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    1.0E+0011  0.000  7300.0  ! MES 738
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    3.0E-0001  4.000  8200.0  ! MES 739
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    2.0E+0011  0.000  9600.0  ! MES 740
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 741
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 742
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    3.0E+0012  0.000  17500.0  ! MES 743
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 744
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 745
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    2.0E+0011  0.000  11000.0  ! MES 746
     DUPLICATE
C3H6Y+B1O=>RC3H5Y+R2OH    1.7E+0011  0.700  5900.0  ! MES 747
C4H8Y+B1O=>RC4H7Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 748
     DUPLICATE
C4H8Y+B1O=>RC4H7Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 749
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 750
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 751
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    7.8E+0013  0.000  5200.0  ! MES 752
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 753
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 754
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    1.0E+0014  0.000  5200.0  ! MES 755
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 756
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 757
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    2.6E+0013  0.000  5200.0  ! MES 758
     DUPLICATE
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! Addition of .Y on YH
RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 759
RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 760
RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 761
RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 762
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y    6.0E+0009  0.000  11400.0  ! ADY 763
RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 764
RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 765
RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 766
RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 767
RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 768
RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 769
RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 770
RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z    6.0E+0009  0.000  11400.0  ! ADY 771
RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 772
RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 773
RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 774
RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z    6.0E+0009  0.000  11400.0  ! ADY 775
RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 776
RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 777
RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 778
RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 779
RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 780
RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 781
RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 782
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 783

! Alkohol reactions
C3H7OH+R1H=>H2+R2OH+C3H6Y    2.9E+0007  2.000  7700.0  ! MOL 784
     DUPLICATE
C3H7OH+R1H=>H2+R2OH+C3H6Y    1.8E+0007  2.000  5000.0  ! MOL 785
     DUPLICATE
C3H7OH+R1H=>H2+R11C2H5+HCHO    2.4E+0006  2.000  6525.0  ! MOL 786
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    2.7E+0006  2.000  450.0  ! MOL 787
     DUPLICATE
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    5.2E+0006  2.000  -765.0  ! MOL 788
     DUPLICATE
C3H7OH+R2OH=>H2O+R11C2H5+HCHO    4.0E+0005  2.000  -475.0  ! MOL 789
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    6.0E+0011  0.000  17000.0  ! MOL 790
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    8.0E+0011  0.000  15500.0  ! MOL 791
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R11C2H5+HCHO    5.4E+0004  2.000  15025.0  ! MOL 792
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    3.0E-0001  4.000  8200.0  ! MOL 793
     DUPLICATE
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    4.0E+0011  0.000  9600.0  ! MOL 794
     DUPLICATE
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO    3.9E+0004  2.000  7525.0  ! MOL 795
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    1.6E+0011  0.000  7300.0  ! MOL 796
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    2.9E+0011  0.000  4500.0  ! MOL 797
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R11C2H5+HCHO    0.0E+0000  0.000  0.0  ! MOL 798
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    3.0E+0011  0.000  13500.0  ! MOL 799
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     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    4.0E+0011  0.000  11000.0  ! MOL 800
     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R11C2H5+HCHO    2.3E+0004  2.000  10525.0  ! MOL 801
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.9E+0007  2.000  7700.0  ! MOL 802
     DUPLICATE
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.7E+0007  2.000  5000.0  ! MOL 803
     DUPLICATE
C4H10OL+R1H=>H2+R19C3H7+HCHO    2.4E+0006  2.000  6525.0  ! MOL 804
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    2.7E+0006  2.000  450.0  ! MOL 805
     DUPLICATE
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    7.8E+0006  2.000  -765.0  ! MOL 806
     DUPLICATE
C4H10OL+R2OH=>H2O+R19C3H7+HCHO    4.0E+0005  2.000  -475.0  ! MOL 807
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    6.0E+0011  0.000  17000.0  ! MOL 808
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    1.2E+0012  0.000  15500.0  ! MOL 809
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R19C3H7+HCHO    5.4E+0004  2.000  15025.0  ! MOL 810
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    3.0E-0001  4.000  8200.0  ! MOL 811
     DUPLICATE
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    6.0E+0011  0.000  9600.0  ! MOL 812
     DUPLICATE
C4H10OL+R4CH3=>CH4+R19C3H7+HCHO    3.9E+0004  2.000  7525.0  ! MOL 813
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    1.6E+0011  0.000  7300.0  ! MOL 814
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    4.4E+0011  0.000  4500.0  ! MOL 815
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R19C3H7+HCHO    0.0E+0000  0.000  0.0  ! MOL 816
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    3.0E+0011  0.000  13500.0  ! MOL 817
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    6.0E+0011  0.000  11000.0  ! MOL 818
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R19C3H7+HCHO    2.3E+0004  2.000  10525.0  ! MOL
819
C5H12OL+R1H=>H2+R2OH+C5H10Z    2.9E+0007  2.000  7700.0  ! MOL 820
     DUPLICATE
C5H12OL+R1H=>H2+R2OH+C5H10Z    3.6E+0007  2.000  5000.0  ! MOL 821
     DUPLICATE
C5H12OL+R1H=>H2+R20C4H9+HCHO    2.4E+0006  2.000  6525.0  ! MOL 822
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    2.7E+0006  2.000  450.0  ! MOL 823
     DUPLICATE
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    1.0E+0007  2.000  -765.0  ! MOL 824
     DUPLICATE
C5H12OL+R2OH=>H2O+R20C4H9+HCHO    4.0E+0005  2.000  -475.0  ! MOL 825
C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    6.0E+0011  0.000  17000.0  ! MOL 826
     DUPLICATE
C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    1.6E+0012  0.000  15500.0  ! MOL 827
     DUPLICATE
C5H12OL+R3OOH=>H2O2+R20C4H9+HCHO    5.4E+0004  2.000  15025.0  ! MOL 828
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    3.0E-0001  4.000  8200.0  ! MOL 829
     DUPLICATE
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    8.0E+0011  0.000  9600.0  ! MOL 830
     DUPLICATE
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C5H12OL+R4CH3=>CH4+R20C4H9+HCHO    3.9E+0004  2.000  7525.0  ! MOL 831
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    1.6E+0011  0.000  7300.0  ! MOL
832
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    5.8E+0011  0.000  4500.0  ! MOL
833
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R20C4H9+HCHO    0.0E+0000  0.000  0.0  ! MOL 834
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    3.0E+0011  0.000  13500.0  ! MOL 835
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    8.0E+0011  0.000  11000.0  ! MOL 836
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R20C4H9+HCHO    2.3E+0004  2.000  10525.0  ! MOL
837
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    3.9E+0013  0.000  5200.0  ! MOL 838
     DUPLICATE
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    4.0E+0013  0.000  5200.0  ! MOL 839
     DUPLICATE
C3H7OH+B1O=>R2OH+R11C2H5+HCHO    1.3E+0006  2.000  5025.0  ! MOL 840
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    3.9E+0013  0.000  5200.0  ! MOL 841
     DUPLICATE
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    6.0E+0013  0.000  5200.0  ! MOL 842
     DUPLICATE
C4H10OL+B1O=>R2OH+R19C3H7+HCHO    1.3E+0006  2.000  5025.0  ! MOL 843
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    3.9E+0013  0.000  5200.0  ! MOL 844
     DUPLICATE
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    8.0E+0013  0.000  5200.0  ! MOL 845
     DUPLICATE
C5H12OL+B1O=>R2OH+R20C4H9+HCHO    1.3E+0006  2.000  5025.0  ! MOL 846

! Aldehydes metathesis
C2H5CHO+R1H=>H2+RC3H5O    4.0E+0013  0.000  4200.0  ! ADZ 847
C2H5CHO+R2OH=>H2O+RC3H5O    4.2E+0012  0.000  500.0  ! ADZ 848
C2H5CHO+R3OOH=>H2O2+RC3H5O    1.0E+0012  0.000  10000.0  ! ADZ 849
C2H5CHO+R4CH3=>CH4+RC3H5O    2.0E-0006  5.600  2500.0  ! ADZ 850
C2H5CHO+R11C2H5=>C2H6+RC3H5O    1.3E+0012  0.000  8500.0  ! ADZ 851
C5H10OA+R1H=>H2+RC5H9O    4.0E+0013  0.000  4200.0  ! ADZ 852
C5H10OA+R2OH=>H2O+RC5H9O    4.2E+0012  0.000  500.0  ! ADZ 853
C5H10OA+R3OOH=>H2O2+RC5H9O    1.0E+0012  0.000  10000.0  ! ADZ 854
C5H10OA+R4CH3=>CH4+RC5H9O    2.0E-0006  5.600  2500.0  ! ADZ 855
C5H10OA+R11C2H5=>C2H6+RC5H9O    1.3E+0012  0.000  8500.0  ! ADZ 856
C4H8OA+R1H=>H2+RC4H7O    4.0E+0013  0.000  4200.0  ! ADZ 857
C4H8OA+R2OH=>H2O+RC4H7O    4.2E+0012  0.000  500.0  ! ADZ 858
C4H8OA+R3OOH=>H2O2+RC4H7O    1.0E+0012  0.000  10000.0  ! ADZ 859
C4H8OA+R4CH3=>CH4+RC4H7O    2.0E-0006  5.600  2500.0  ! ADZ 860
C4H8OA+R11C2H5=>C2H6+RC4H7O    1.3E+0012  0.000  8500.0  ! ADZ 861
C6H12OA+R1H=>H2+RC6H11O    4.0E+0013  0.000  4200.0  ! ADZ 862
C6H12OA+R2OH=>H2O+RC6H11O    4.2E+0012  0.000  500.0  ! ADZ 863
C6H12OA+R3OOH=>H2O2+RC6H11O    1.0E+0012  0.000  10000.0  ! ADZ 864
C6H12OA+R4CH3=>CH4+RC6H11O    2.0E-0006  5.600  2500.0  ! ADZ 865
C6H12OA+R11C2H5=>C2H6+RC6H11O    1.3E+0012  0.000  8500.0  ! ADZ 866
C7H14OA+R1H=>H2+RC7H13O    4.0E+0013  0.000  4200.0  ! ADZ 867
C7H14OA+R2OH=>H2O+RC7H13O    4.2E+0012  0.000  500.0  ! ADZ 868
C7H14OA+R3OOH=>H2O2+RC7H13O    1.0E+0012  0.000  10000.0  ! ADZ 869
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C7H14OA+R4CH3=>CH4+RC7H13O    2.0E-0006  5.600  2500.0  ! ADZ 870
C7H14OA+R11C2H5=>C2H6+RC7H13O    1.3E+0012  0.000  8500.0  ! ADZ 871
C8H16OA+R1H=>H2+RC8H15O    4.0E+0013  0.000  4200.0  ! ADZ 872
C8H16OA+R2OH=>H2O+RC8H15O    4.2E+0012  0.000  500.0  ! ADZ 873
C8H16OA+R3OOH=>H2O2+RC8H15O    1.0E+0012  0.000  10000.0  ! ADZ 874
C8H16OA+R4CH3=>CH4+RC8H15O    2.0E-0006  5.600  2500.0  ! ADZ 875
C8H16OA+R11C2H5=>C2H6+RC8H15O    1.3E+0012  0.000  8500.0  ! ADZ 876
C9H18OA+R1H=>H2+RC9H17O    4.0E+0013  0.000  4200.0  ! ADZ 877
C9H18OA+R2OH=>H2O+RC9H17O    4.2E+0012  0.000  500.0  ! ADZ 878
C9H18OA+R3OOH=>H2O2+RC9H17O    1.0E+0012  0.000  10000.0  ! ADZ 879
C9H18OA+R4CH3=>CH4+RC9H17O    2.0E-0006  5.600  2500.0  ! ADZ 880
C9H18OA+R11C2H5=>C2H6+RC9H17O    1.3E+0012  0.000  8500.0  ! ADZ 881
C12H24OA+R1H=>H2+RC12H23O    4.0E+0013  0.000  4200.0  ! ADZ 882
C12H24OA+R2OH=>H2O+RC12H23O    4.2E+0012  0.000  500.0  ! ADZ 883
C12H24OA+R3OOH=>H2O2+RC12H23O    1.0E+0012  0.000  10000.0  ! ADZ 884
C12H24OA+R4CH3=>CH4+RC12H23O    2.0E-0006  5.600  2500.0  ! ADZ 885
C12H24OA+R11C2H5=>C2H6+RC12H23O    1.3E+0012  0.000  8500.0  ! ADZ 886
C11H22OA+R1H=>H2+RC11H21O    4.0E+0013  0.000  4200.0  ! ADZ 887
C11H22OA+R2OH=>H2O+RC11H21O    4.2E+0012  0.000  500.0  ! ADZ 888
C11H22OA+R3OOH=>H2O2+RC11H21O    1.0E+0012  0.000  10000.0  ! ADZ 889
C11H22OA+R4CH3=>CH4+RC11H21O    2.0E-0006  5.600  2500.0  ! ADZ 890
C11H22OA+R11C2H5=>C2H6+RC11H21O    1.3E+0012  0.000  8500.0  ! ADZ 891
C10H20OA+R1H=>H2+RC10H19O    4.0E+0013  0.000  4200.0  ! ADZ 892
C10H20OA+R2OH=>H2O+RC10H19O    4.2E+0012  0.000  500.0  ! ADZ 893
C10H20OA+R3OOH=>H2O2+RC10H19O    1.0E+0012  0.000  10000.0  ! ADZ 894
C10H20OA+R4CH3=>CH4+RC10H19O    2.0E-0006  5.600  2500.0  ! ADZ 895
C10H20OA+R11C2H5=>C2H6+RC10H19O    1.3E+0012  0.000  8500.0  ! ADZ 896
C13H26OA+R1H=>H2+RC13H25O    4.0E+0013  0.000  4200.0  ! ADZ 897
C13H26OA+R2OH=>H2O+RC13H25O    4.2E+0012  0.000  500.0  ! ADZ 898
C13H26OA+R3OOH=>H2O2+RC13H25O    1.0E+0012  0.000  10000.0  ! ADZ 899
C13H26OA+R4CH3=>CH4+RC13H25O    2.0E-0006  5.600  2500.0  ! ADZ 900
C13H26OA+R11C2H5=>C2H6+RC13H25O    1.3E+0012  0.000  8500.0  ! ADZ 901

C4H6OAY+R1H=>H2+R10C2H3V+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 902
C4H6OAY+R2OH=>H2O+R10C2H3V+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 903
C4H6OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ
904
C4H6OAY+R4CH3=>CH4+R10C2H3V+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 905
C4H6OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
906
C5H8OAY+R1H=>H2+RC3H5Y+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 907
C5H8OAY+R2OH=>H2O+RC3H5Y+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 908
C5H8OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ 909
C5H8OAY+R4CH3=>CH4+RC3H5Y+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 910
C5H8OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
911
!C8H14OAY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 912
!C8H14OAY+R2OH=>H2O+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 913
!C8H14OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+2C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 914
!C8H14OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z    2.0E-0006  0.000
2500.0  ! ADZ 915
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!C8H14OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z    1.3E+0012  0.000
8500.0  ! ADZ 916
!C9H16OAY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  ! ADZ
917
!C9H16OAY+R2OH=>H2O+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 918
!C9H16OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ+2C2H4Z    1.0E+0012  0.000
10000.0  ! ADZ 919
!C9H16OAY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 920
!C9H16OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 921
!C6H10OAY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 922
!C6H10OAY+R2OH=>H2O+R10C2H3V+CH2COZ+C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 923
!C6H10OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 924
!C6H10OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 925
!C6H10OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 926

! Keto radicals decomposition
RC3H5O=>B2CO+R11C2H5    1.8E+0014  0.000  15600.0  ! COR 927
RC5H9O=>B2CO+R20C4H9    1.8E+0014  0.000  15600.0  ! COR 928
RC4H7O=>B2CO+R19C3H7    1.8E+0014  0.000  15600.0  ! COR 929
RC6H11O=>B2CO+R35C5H11    1.8E+0014  0.000  15600.0  ! COR 930
RC7H13O=>B2CO+R41C6H13    1.8E+0014  0.000  15600.0  ! COR 931
RC8H15O=>B2CO+R26C7H15    1.8E+0014  0.000  15600.0  ! COR 932
RC9H17O=>B2CO+R30C8H17    1.8E+0014  0.000  15600.0  ! COR 933
RC12H23O=>B2CO+R4CH3+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 934
RC11H21O=>B2CO+R11C2H5+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 935
RC10H19O=>B2CO+R4CH3+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 936
RC13H25O=>B2CO+R11C2H5+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 937


! keto radicals addition to O2
RC3H5O+O2=>RC3H5O3    3.0E+0019  -2.500  0.0  ! COR 938
RC5H9O+O2=>RC5H9O3    3.0E+0019  -2.500  0.0  ! COR 939
RC4H7O+O2=>RC4H7O3    3.0E+0019  -2.500  0.0  ! COR 940
RC6H11O+O2=>RC6H11O3    3.0E+0019  -2.500  0.0  ! COR 941
RC7H13O+O2=>RC7H13O3    3.0E+0019  -2.500  0.0  ! COR 942
RC8H15O+O2=>RC8H15O3    3.0E+0019  -2.500  0.0  ! COR 943
RC9H17O+O2=>RC9H17O3    3.0E+0019  -2.500  0.0  ! COR 944
RC12H23O+O2=>RC12H23O3    3.0E+0019  -2.500  0.0  ! COR 945
RC11H21O+O2=>RC11H21O3    3.0E+0019  -2.500  0.0  ! COR 946
RC10H19O+O2=>RC10H19O3    3.0E+0019  -2.500  0.0  ! COR 947
RC13H25O+O2=>RC13H25O3    3.0E+0019  -2.500  0.0  ! COR 948

! Peracide radical decomposition
RC3H5O3=>C2H4Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 949
RC5H9O3=>C4H8Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 950
RC4H7O3=>C3H6Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 951
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RC6H11O3=>C5H10Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 952
RC7H13O3=>C6H12Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 953
RC8H15O3=>C7H14Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 954
RC9H17O3=>C8H16Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 955
RC12H23O3=>C11H22Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 956
RC11H21O3=>C10H20Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 957
RC10H19O3=>C9H18Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 958
RC13H25O3=>C12H24Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 959

! Ketones reactions
!C2H6CO+R1H=>H2+CH2COZ+R4CH3    5.7E+0007  2.000  7700.0  ! MK 960
!C2H6CO+R2OH=>H2O+CH2COZ+R4CH3    5.4E+0006  2.000  450.0  ! MK 961
!C2H6CO+R3OOH=>H2O2+CH2COZ+R4CH3    1.2E+0012  0.000  17000.0  ! MK 962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3    6.0E-0001  4.000  8200.0  ! MK 963
!C2H6CO+R8CH3OO=>CH3OOH+CH2COZ+R4CH3    1.2E+0013  0.000  20000.0  ! MK
964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3    6.0E+0011  0.000  13500.0  ! MK 965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    5.7E+0007  2.000  7700.0  ! MK 966
     DUPLICATE
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    9.0E+0006  2.000  5000.0  ! MK 967
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    5.4E+0006  2.000  450.0  ! MK 968
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    2.6E+0006  2.000  -765.0  ! MK 969
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    1.2E+0012  0.000  17000.0  ! MK 970
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    4.0E+0011  0.000  15500.0  ! MK 971
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    6.0E-0001  4.000  8200.0  ! MK 972
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    2.0E+0011  0.000  9600.0  ! MK 973
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    1.2E+0013  0.000  20000.0  ! MK
974
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    3.0E+0012  0.000  17500.0  ! MK
975
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    6.0E+0011  0.000  13500.0  ! MK
976
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    2.0E+0011  0.000  11000.0  ! MK
977
     DUPLICATE



! Unsaturated ester reactions
! Esters metatesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis
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! Addition on unsaturated esters

! Carboxylic acid reactions
! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alkohol ene to dienes
C3H6OLY+R1H=>H2+HCHO+R10C2H3V    5.4E+0004  2.500  -1900.0  ! ROH 978
C3H6OLY+R2OH=>H2O+HCHO+R10C2H3V    3.0E+0006  2.000  -1520.0  ! ROH 979
C3H6OLY+R3OOH=>H2O2+HCHO+R10C2H3V    6.4E+0003  2.600  12400.0  ! ROH 980
C3H6OLY+R4CH3=>CH4+HCHO+R10C2H3V    1.0E+0011  0.000  7300.0  ! ROH 981
C3H6OLY+R8CH3OO=>CH3OOH+HCHO+R10C2H3V    1.0E+0012  0.000  14550.0  ! ROH
982
C3H6OLY+R11C2H5=>C2H6+HCHO+R10C2H3V    1.5E+0000  3.500  4140.0  ! ROH
983
C4H8OLY+R1H=>H2+HCHO+RC3H5Y    5.4E+0004  2.500  -1900.0  ! ROH 984
C4H8OLY+R2OH=>H2O+HCHO+RC3H5Y    3.0E+0006  2.000  -1520.0  ! ROH 985
C4H8OLY+R3OOH=>H2O2+HCHO+RC3H5Y    6.4E+0003  2.600  12400.0  ! ROH 986
C4H8OLY+R4CH3=>CH4+HCHO+RC3H5Y    1.0E+0011  0.000  7300.0  ! ROH 987
C4H8OLY+R8CH3OO=>CH3OOH+HCHO+RC3H5Y    1.0E+0012  0.000  14550.0  ! ROH
988
C4H8OLY+R11C2H5=>C2H6+HCHO+RC3H5Y    1.5E+0000  3.500  4140.0  ! ROH 989
C5H10OLY+R1H=>H2+HCHO+RC4H7Y    5.4E+0004  2.500  -1900.0  ! ROH 990
C5H10OLY+R2OH=>H2O+HCHO+RC4H7Y    3.0E+0006  2.000  -1520.0  ! ROH 991
C5H10OLY+R3OOH=>H2O2+HCHO+RC4H7Y    6.4E+0003  2.600  12400.0  ! ROH 992
C5H10OLY+R4CH3=>CH4+HCHO+RC4H7Y    1.0E+0011  0.000  7300.0  ! ROH 993
C5H10OLY+R8CH3OO=>CH3OOH+HCHO+RC4H7Y    1.0E+0012  0.000  14550.0  ! ROH
994
C5H10OLY+R11C2H5=>C2H6+HCHO+RC4H7Y    1.5E+0000  3.500  4140.0  ! ROH 995
C7H14OLY+R1H=>H2+HCHO+RC6H11Y    5.4E+0004  2.500  -1900.0  ! ROH 996
C7H14OLY+R2OH=>H2O+HCHO+RC6H11Y    3.0E+0006  2.000  -1520.0  ! ROH 997
C7H14OLY+R3OOH=>H2O2+HCHO+RC6H11Y    6.4E+0003  2.600  12400.0  ! ROH 998
C7H14OLY+R4CH3=>CH4+HCHO+RC6H11Y    1.0E+0011  0.000  7300.0  ! ROH 999
C7H14OLY+R8CH3OO=>CH3OOH+HCHO+RC6H11Y    1.0E+0012  0.000  14550.0  ! ROH
1000
C7H14OLY+R11C2H5=>C2H6+HCHO+RC6H11Y    1.5E+0000  3.500  4140.0  ! ROH
1001
C8H16OLY+R1H=>H2+HCHO+RC7H13Y    5.4E+0004  2.500  -1900.0  ! ROH 1002
C8H16OLY+R2OH=>H2O+HCHO+RC7H13Y    3.0E+0006  2.000  -1520.0  ! ROH 1003
C8H16OLY+R3OOH=>H2O2+HCHO+RC7H13Y    6.4E+0003  2.600  12400.0  ! ROH
1004
C8H16OLY+R4CH3=>CH4+HCHO+RC7H13Y    1.0E+0011  0.000  7300.0  ! ROH 1005
C8H16OLY+R8CH3OO=>CH3OOH+HCHO+RC7H13Y    1.0E+0012  0.000  14550.0  ! ROH
1006
C8H16OLY+R11C2H5=>C2H6+HCHO+RC7H13Y    1.5E+0000  3.500  4140.0  ! ROH
1007
C9H18OLY+R1H=>H2+HCHO+RC8H15Y    5.4E+0004  2.500  -1900.0  ! ROH 1008
C9H18OLY+R2OH=>H2O+HCHO+RC8H15Y    3.0E+0006  2.000  -1520.0  ! ROH 1009
C9H18OLY+R3OOH=>H2O2+HCHO+RC8H15Y    6.4E+0003  2.600  12400.0  ! ROH
1010
C9H18OLY+R4CH3=>CH4+HCHO+RC8H15Y    1.0E+0011  0.000  7300.0  ! ROH 1011
C9H18OLY+R8CH3OO=>CH3OOH+HCHO+RC8H15Y    1.0E+0012  0.000  14550.0  ! ROH
1012
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C9H18OLY+R11C2H5=>C2H6+HCHO+RC8H15Y    1.5E+0000  3.500  4140.0  ! ROH
1013
C6H12OLY+R1H=>H2+HCHO+RC5H9Y    5.4E+0004  2.500  -1900.0  ! ROH 1014
C6H12OLY+R2OH=>H2O+HCHO+RC5H9Y    3.0E+0006  2.000  -1520.0  ! ROH 1015
C6H12OLY+R3OOH=>H2O2+HCHO+RC5H9Y    6.4E+0003  2.600  12400.0  ! ROH 1016
C6H12OLY+R4CH3=>CH4+HCHO+RC5H9Y    1.0E+0011  0.000  7300.0  ! ROH 1017
C6H12OLY+R8CH3OO=>CH3OOH+HCHO+RC5H9Y    1.0E+0012  0.000  14550.0  ! ROH
1018
C6H12OLY+R11C2H5=>C2H6+HCHO+RC5H9Y    1.5E+0000  3.500  4140.0  ! ROH
1019

! Additions on dienes
C4H6Z2+R2OH=>RC3H5Y+HCHO    1.4E+0012  0.000  -1040.0  ! AD 1020!!!!!!ds
мйса toluиne
!
!C4H6Z2+R2OH=>RC3H5Y+HCHO    3.0E+0012  0.000  -1040.0  !
!
C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V    1.0E+0005  2.500  -1900.0  ! AD 1021
C6H10Y2+R2OH=>H2O+C4H6Z2+R10C2H3V    6.0E+0006  2.000  -1520.0  ! AD 1022
C6H10Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V    1.2E+0004  2.600  12400.0  ! AD
1023
C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD 1024
C6H10Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD
1025
C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V    3.0E+0000  3.500  4140.0  ! AD
1026
C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y    1.0E+0005  2.500  -1900.0  ! AD 1027
C7H12Y2+R2OH=>H2O+C4H6Z2+RC3H5Y    6.0E+0006  2.000  -1520.0  ! AD 1028
C7H12Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y    1.2E+0004  2.600  12400.0  ! AD 1029
C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD 1030
C7H12Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD
1031
C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y    3.0E+0000  3.500  4140.0  ! AD
1032
!C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1033
!C10H18Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+2C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1034
!C10H18Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z    1.2E+0004  2.600  12400.0
! AD 1035
!C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1036
!C10H18Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1037
!C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1038
!C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1039
!C11H20Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+2C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1040
!C11H20Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1041
!C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1042
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!C11H20Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1043
!C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z    3.0E+0000  3.500  4140.0
! AD 1044
!C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1045
!C8H14Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1046
!C8H14Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1047
!C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1048
!C8H14Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1049
!C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z    3.0E+0000  3.500  4140.0
! AD 1050
!C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1051
!C12H22Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+3C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1052
!C12H22Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+3C2H4Z    1.2E+0004  2.600  12400.0
! AD 1053
!C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1054
!C12H22Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1055
!C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1056
!C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1057
!C9H16Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+C2H4Z    6.0E+0006  2.000  -1520.0  ! AD
1058
!C9H16Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+C2H4Z    1.2E+0004  2.600  12400.0  !
AD 1059
!C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0  ! AD
1060
!C9H16Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0
! AD 1061
!C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z    3.0E+0000  3.500  4140.0  !
AD 1062
!C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1063
!C14H26Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+4C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1064
!C14H26Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+4C2H4Z    1.2E+0004  2.600  12400.0
! AD 1065
!C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1066
!C14H26Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1067
!C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1068
!C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1069
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!C15H28Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+4C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1070
!C15H28Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+4C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1071
!C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1072
!C15H28Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1073
!C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z    3.0E+0000  3.500  4140.0
! AD 1074
!C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1075
!C16H30Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+5C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1076
!C16H30Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+5C2H4Z    1.2E+0004  2.600  12400.0
! AD 1077
!C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1078
!C16H30Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1079
!C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1080
!C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1081
!C13H24Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+3C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1082
!C13H24Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+3C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1083
!C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1084
!C13H24Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1085
!C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z    3.0E+0000  3.500  4140.0
! AD 1086

! Diels Alder

! .Y termination
RC3H5Y+R1H=>C3H6Y    1.0E+0014  0.000  0.0  ! TER
1087 !!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC3H5Y+R2OH=>C3H6OLY    1.0E+0013  0.000  0.0  ! TER 1088
RC3H5Y+R3OOH=>C3H6O2PY    5.0E+0012  0.000  0.0  ! TER 1089
RC3H5Y+R4CH3=>C4H8Y    1.0E+0013  0.000  0.0  ! TER 1090
RC3H5Y+R5CHO=>C4H6OAY    1.0E+0013  0.000  0.0  ! TER 1091
RC3H5Y+R6CH2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1092
RC3H5Y+R8CH3OO=>HCHO+R7CH3O+R10C2H3V    1.0E+0013  0.000  0.0  ! TER 1093
RC3H5Y+R11C2H5=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1094
RC4H7Y+R1H=>C4H8Y    1.0E+0014  0.000  0.0  ! TER
1095!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC4H7Y+R2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1096
RC4H7Y+R3OOH=>C4H8O2PY    5.0E+0012  0.000  0.0  ! TER 1097
RC4H7Y+R4CH3=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1098
RC4H7Y+R5CHO=>C5H8OAY    1.0E+0013  0.000  0.0  ! TER 1099
RC4H7Y+R6CH2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1100
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RC4H7Y+R8CH3OO=>HCHO+R7CH3O+RC3H5Y    1.0E+0013  0.000  0.0  ! TER 1101
RC4H7Y+R11C2H5=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1102
RC7H13Y+R1H=>C7H14Y    1.0E+0014  0.000  0.0  ! TER
1103!!!!!!!!!!!!!!!!!!!!multiplій x10
RC7H13Y+R2OH=>C7H14OLY    1.0E+0013  0.000  0.0  ! TER 1104
RC7H13Y+R3OOH=>C7H14O2PY    5.0E+0012  0.000  0.0  ! TER 1105
RC7H13Y+R4CH3=>C8H16Y    1.0E+0013  0.000  0.0  ! TER 1106
RC7H13Y+R5CHO=>C8H14OAY    1.0E+0013  0.000  0.0  ! TER 1107
RC7H13Y+R6CH2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1108
RC7H13Y+R8CH3OO=>HCHO+R7CH3O+RC6H11Y    1.0E+0013  0.000  0.0  ! TER 1109
RC7H13Y+R11C2H5=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1110
RC8H15Y+R1H=>C8H16Y    1.0E+0014  0.000  0.0  ! TER
1111!!!!!!!!!!!!!!!!!!!!multiplій x10
RC8H15Y+R2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1112
RC8H15Y+R3OOH=>C8H16O2PY    5.0E+0012  0.000  0.0  ! TER 1113
RC8H15Y+R4CH3=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1114
RC8H15Y+R5CHO=>C9H16OAY    1.0E+0013  0.000  0.0  ! TER 1115
RC8H15Y+R6CH2OH=>C9H18OLY    1.0E+0013  0.000  0.0  ! TER 1116
RC8H15Y+R8CH3OO=>HCHO+R7CH3O+RC7H13Y    1.0E+0013  0.000  0.0  ! TER 1117
RC8H15Y+R11C2H5=>C10H20Z    1.0E+0013  0.000  0.0  ! TER 1118
RC5H9Y+R1H=>C5H10Y    1.0E+0014  0.000  0.0  ! TER
1119!!!!!!!!!!!!!!!!!!!!multiplій x10
RC5H9Y+R2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1120
RC5H9Y+R3OOH=>C5H10O2PY    5.0E+0012  0.000  0.0  ! TER 1121
RC5H9Y+R4CH3=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1122
RC5H9Y+R5CHO=>C6H10OAY    1.0E+0013  0.000  0.0  ! TER 1123
RC5H9Y+R6CH2OH=>C6H12OLY    1.0E+0013  0.000  0.0  ! TER 1124
RC5H9Y+R8CH3OO=>HCHO+R7CH3O+RC4H7Y    1.0E+0013  0.000  0.0  ! TER 1125
RC5H9Y+R11C2H5=>C7H14Y    1.0E+0013  0.000  0.0  ! TER 1126
RC3H5Y+RC3H5Y=>C6H10Y2    1.0E+0013  0.000  0.0  ! TER 1127
RC3H5Y+RC4H7Y=>C7H12Y2    1.0E+0013  0.000  0.0  ! TER 1128
RC3H5Y+RC7H13Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1129
RC3H5Y+RC8H15Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1130
RC3H5Y+RC5H9Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1131
RC4H7Y+RC4H7Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1132
RC4H7Y+RC7H13Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1133
RC4H7Y+RC8H15Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1134
RC4H7Y+RC5H9Y=>C9H16Y2    1.0E+0013  0.000  0.0  ! TER 1135
RC7H13Y+RC7H13Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1136
RC7H13Y+RC8H15Y=>C15H28Y2    1.0E+0013  0.000  0.0  ! TER 1137
RC7H13Y+RC5H9Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1138
RC8H15Y+RC8H15Y=>C16H30Y2    1.0E+0013  0.000  0.0  ! TER 1139
RC8H15Y+RC5H9Y=>C13H24Y2    1.0E+0013  0.000  0.0  ! TER 1140
RC8H15Y+RC6H11Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1141
RC5H9Y+RC5H9Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1142
RC5H9Y+RC6H11Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1143

!
**********************************************************************
**!
!especes excitees!
R1H+B1O+M=OHE+M                  6.0E14      0.0      6.94E3     !
<HALL05>!
```

```
B4CH+O2=B2CO+OHE                  4.0E13      0.0      0.0        !
<HALL05>!
OHE+AR=R2OH+AR                    5.2E10      0.5      0.0        !
<HALL05>!
OHE+H2O=R2OH+H2O                  8.6E12      0.5      0.0        !
<HALL05>!
OHE+H2=R2OH+H2                    1.5E12      0.5      0.0        !
<HALL05>!
OHE+R1H=R2OH+R1H                  1.5E12      0.5      0.0        !
<HALL05>!
OHE+O2=R2OH+O2                    1.5E12      0.5      0.0        !
<HALL05>!
OHE+B1O=R2OH+B1O                  1.5E12      0.5      0.0        !
<HALL05>!
OHE+R2OH=R2OH+R2OH                1.5E12      0.5      0.0        !
<HALL05>!
OHE=>R2OH                            1.4E6       0.0      0.0        !
<HALL05>!
OHE+CO2=R2OH+CO2                  2.75E12     0.5     -968.      !
<HALL05>!
OHE+B2CO=R2OH+B2CO                3.23E12     0.5     -787.      !
<HALL05>!
OHE+CH4=R2OH+CH4                  3.36E12     0.5     -635.      !
<HALL05>!
R9C2H+B1O=B2CO+CHE                6.2E12      0.0      0.0        !
<HALL05>!
R9C2H+O2=CO2+CHE                  2.17E10     0.0      0.0        !
<HALL05>!
CHE+AR=B4CH+AR                    4.0E10      0.5      0.0        !
<HALL05>!
CHE+O2=B4CH+O2                    2.48E6      2.14     0.0        !
<HALL05>!
CHE+H2O=B4CH+H2O                  5.3E13      0.0      0.0        !
<HALL05>!
CHE+H2=B4CH+H2                    1.47E14     0.0      1360.      !
<HALL05>!
CHE+CO2=B4CH+CO2                  2.41E-1     4.3     -1694.          !
<HALL05>!
CHE+B2CO=B4CH+B2CO                2.44E12     0.5      0.0       !
<HALL05>!
CHE+CH4=B4CH+CH4                  1.73E13     0.0      167.      !
<HALL05>!
CHE=>B4CH                            1.86E6      0.0      0.0        !
<HALL05>!


!*******************************************!
!     REACTIONS DE LA MATRICE O(0)C(y)H(z)   !
!*******************************************!

!****** REACTIONS DE H2******!
R1H+R1H+M=H2+M                1.87E18     -1.00     0.00
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/
AR/0.35/
```

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!      N2/0.4/ HE/0.35/

!****** REACTIONS DE B4CH ******!
B4CH+R1H=B3C+H2             7.8E13       0.       0.       !(2,-
2)<PEETERS97>!

!****** REACTIONS DE B6CH2 ******!
B6CH2+M=B5CH2+M              1.51E13      0.0      0.0
       O2/.4/ B2CO/.75/ CO2/1.5/ H2O/6.5/ CH4/.48/  C2H4Z/1.6/
      AR/.24/
B6CH2+R1H=B4CH+H2            3.0E13       0.       0.           !(4,-
4)<TSAnG86>!

!****** REACTIONS DE B5CH2 ******!
B5CH2+R1H=B4CH+H2            6.0E12       0.      -1.8E3        !(5,-
5)<BAULCH94>!
B5CH2+B3C=R9C2H+R1H         5.0E13       0.       0.           !(6,-
6)<RAnZI94>!
B5CH2+B5CH2=>C2H2+R1H+R1H    1.2E14       0.       0.8E3        !
(7)<BAULCH94>!

!****** REACTIONS DE R4CH3 ******!
R4CH3+M=B5CH2+R1H+M              2.91E16     0.0     90.7E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R4CH3+R1H=B6CH2+H2            6.0E13      0.        15.0E3           !
(9,-9)<BAULCH94>!
R4CH3+B4CH=R10C2H3V+R1H       3.0E13      0.         0.          !(10,-
10)<DAGAUT91>
R4CH3+B6CH2=C2H4Z+R1H         1.8E13      0.         0.          !(11,-
11)<TSAnG86>!
R4CH3+B5CH2=C2H4Z+R1H         4.2E13      0.         0.          !(12,-
12)<BAULCH94>!
R4CH3+B3C=C2H2+R1H           5.0E13      0.         0.           !(13,-
13)<RAnZI94>!
R4CH3+R4CH3(+M)=>C2H6(+M)     3.61E13     0.         0.          !
(14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.63E41  -7.0   2.76E3 /
      TROE /  0.62  73  1180 /
C2H6(+M)=>R4CH3+R4CH3(+M)     1.8E21      -1.24    90.9E3        !(-
14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 1.89E49   -8.24   93.7E3/
      TROE /  0.62  73  1180 /
R4CH3+R4CH3=R11C2H5+R1H        3.0E13      0.      13.5E3        !(15,-
15)<BAULCH94>!
R4CH3+R4CH3=C2H4Z+H2           2.1E14      0.      19.3E3        !(16,-
16)<FRAnK86nIST>!

!****** REACTIONS DE CH4 ******!
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R1H+R4CH3(+M)=>CH4(+M)        1.67E14     0.      0.             !
(17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW /  1.408E24  -1.8   0.0 /
      TROE / 0.37 3315 61 /
CH4(+M)=>R4CH3+R1H(+M)        2.4E16      0.    105.0E3          !(-
17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/
!     N2/0.4/ HE/0.35/
      LOW / 1.29E18    0.00  90.9E3 /
      TROE / 0  1350  1  7830 /
CH4(+CH4)=>R4CH3+R1H(+CH4)    2.4E16      0.    105.0E3          !(-
17')<BAULCH94>!
      LOW / 8.43E17    0.00  90.9E3 /
      TROE / 0.69  90  2210 /
CH4+R1H=R4CH3+H2              1.3E04      3.      8.0E3          !(18,-
18)<BAULCH94>!
CH4+B4CH=C2H4Z+R1H            3.0E13      0.     -0.4E3          !(19,-
19)<DAGAUT91BAULCH94>!
CH4+B6CH2=R4CH3+R4CH3         4.2E13      0.      0.             !(20,-
20)<TSAnG86>!

!****** REACTIONS DE R9C2H ******!
R9C2H+B6CH2=C2H2+B4CH         1.8E13      0.         0.          !(21,-
21)<TSAnG86>!
R9C2H+B5CH2=C2H2+B4CH         1.8E13      0.         0.          !(22,-
22)<TSAnG86>!
R9C2H+CH4=C2H2+R4CH3          1.2E12      0.         0.          !(23,-
23)<BAULCH94>!

!****** REACTIONS DE C2H2 ******!
C2H2+M=R9C2H+R1H+M            1.14E17     0.    107.0E3          !(24,-
24)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H2+R1H=R9C2H+H2             6.6E13      0.     27.7E3          !(25,-
25)<BAULCH94>!

!****** REACTIONS DE R10C2H3V ******!
R10C2H3V(+M)=C2H2+R1H(+M)     2.0E14      0.     39.8E3          !(26,-
26)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 1.19E42  -7.50  45.55E3 /
      TROE    /0.35   1.0       1.E8/
R10C2H3V+R1H=C2H2+H2          1.2E13      0.         0.          !(27,-
27)<BAULCH94>!
R10C2H3V+B6CH2=C2H2+R4CH3     1.8E13      0.         0.          !(28,-
28)<TSAnG86>!
R10C2H3V+B5CH2=C2H2+R4CH3     1.8E13      0.         0.          !(29,-
29)<TSAnG86>!
R10C2H3V+R4CH3=CH4+C2H2       3.9E11      0.         0.          !(30,-
30)<TSAnG86>!
```

```
R10C2H3V+R9C2H=2C2H2          9.6E11      0.          0.          !(31,-
31)<TSAnG86>!
R10C2H3V+R10C2H3V=C2H4Z+C2H2  9.6E11      0.          0.          !(32,-
32)<TSAnG86>!

!****** REACTIONS DE C2H4Z ******!
C2H4Z+M=C2H2+H2+M             9.97E16     0.     71.6E3           !(33,-
33)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H4Z+M=R10C2H3V+R1H+M        7.40E17     0.     96.7E3           !(34,-
34)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!C2H4Z+R1H=R10C2H3V+H2         5.4E14      0.     14.8E3           !(35,-
35)<BAULCH94>!
C2H4Z+R1H=R10C2H3V+H2         5.0E7       1.93   13.0E3           !(35,-
35)SLAGLE96!
!C2H4Z+R4CH3=CH4+R10C2H3V     4.1E12      0.     11.1E3           !(36,-
36)<BAULCH94>!
C2H4Z+R4CH3=CH4+R10C2H3V      6.3E11      0.     16.0E3           !(36,-
36)BACK89!

!****** REACTIONS DE R11C2H5 ******!
!C2H4Z+R1H(+M)=>R11C2H5(+M)    3.97E09    1.28     1.3E3
!      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!      LOW / 1.35E19   0.00   0.76E3 /
!      TROE / 0.76  40  1025/
R11C2H5(+M)=C2H4Z+R1H(+M)      8.2E13      0.    40.0E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.40E17   0.00   33.4E3 /
      TROE / 0.75  97  1379/
R11C2H5+R1H=C2H4Z+H2           1.8E12      0.          0.          !(38,-
38)<TSAnG86>!
R11C2H5+R1H=C2H6               3.6E13      0.          0.          !(39,-
39><TSAnG86>!
R11C2H5+B6CH2=C2H4Z+R4CH3      9.0E12      0.          0.          !(40,-
40)<TSAnG86>!
R11C2H5+B5CH2=C2H4Z+R4CH3      1.8E13      0.          0.          !(41,-
41)<TSAnG86>!
R11C2H5+R4CH3=C2H4Z+CH4        1.1E12      0.          0.          !(42,-
42)<BAULCH94>!
R11C2H5+R9C2H=C2H2+C2H4Z       1.8E12      0           0.          !(43,-
43)<TSAnG86>!
R11C2H5+R10C2H3V=2C2H4Z        4.8E11      0.          0.          !(44,-
44)<TSAnG86>!
R11C2H5+R10C2H3V=C2H2+C2H6     4.8E11      0.          0.          !(45,-
45)<TSAnG86>!
R11C2H5+R11C2H5=C2H4Z+C2H6     1.4E12      0.          0.          !(46,-
46)<BAULCH94>!

!****** REACTIONS DE C2H6 ******!
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```
C2H6+M=C2H4Z+H2+M              2.3E17      0.     67.4E3        !(47,-
47)<SCHULTZ85nIST>!
C2H6+R1H=R11C2H5+H2            1.4E9       1.5     7.4E3        !(48,-
48)<BAULCH94>!
C2H6+B6CH2=R4CH3+R11C2H5       1.1E14      0.        0.         !(49,-
49)<TSAnG86>!
C2H6+R4CH3=R11C2H5+CH4         1.5E-7      6.0     5.8E3        !(50,-
50)<BAULCH94>!
C2H6+R9C2H=C2H2+R11C2H5        3.6E12      0.        0.         !(51,-
51)<TSAnG86>!
C2H6+R10C2H3V=R11C2H5+C2H4Z    6.0E2       3.3    10.5E3        !(52,-
52)<TSAnG86>!


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!*****************************************************!
!          REACTIONS DE LA MATRICE O(x)C(y)H(z)  x>0      !
!*****************************************************!

!****** REACTIONS DE B1O ******!
B1O+H2=R2OH+R1H                5.1E4       2.67    6.2E3        !(53,-
53)<BAULCH94>!
B1O+B4CH=B2CO+R1H              3.9E13      0.        0.         !(54,-
54)<BAULCH94>!
B1O+B4CH=B3C+R2OH             1.5E13      0.     4.7E3         !(55,-
55)<MUR86nIS>!
B1O+B6CH2=>B2CO+2R1H           1.5E13      0.        0.         !(56)
<TSAnG86>!
B1O+B6CH2=B2CO+H2              1.5E13      0.        0.         !(57,-57)
<TSAnG86>!
B1O+B5CH2=>B2CO+2R1H           7.2E13      0.        0.         !(58)
<BAULCH94>!
B1O+B5CH2=B2CO+H2              4.8E13      0.        0.         !(59,-
59)<BAULCH94>!
B1O+R4CH3=HCHO+R1H             8.4E13      0.        0.         !(60,-
60)<BAULCH94>!
B1O+R4CH3=R7CH3O               8.0E15     -2.12    0.6E3        !(61,-
61)<DEAn87nIS>!
B1O+CH4=R4CH3+R2OH             7.2E8       1.56    8.4E3        !(62,-
62)<BAULCH94>!
B1O+R9C2H=B4CH+B2CO            1.0E13      0.        0.         !(63,-
63)<DAGAUT91>!
B1O+C2H2=B5CH2+B2CO            2.17E06     2.1     1.6E3        !(64,-
64)<BAULCH LEEDS>!
B1O+C2H2=R12CHCOZ+R1H          5.06E06     2.1     1.6E3        !(65,-
65)<BAULCH LEEDS>!
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R2OH+R9C2H=C2H2+B1O             1.8E13      0.          0.        !(89,-
89)<TSANG86>! modif MF
B1O+R10C2H3V=R4CH3+B2CO         3.0E13      0.          0.        !(66,-
66)<DAGAUT91>!
B1O+R10C2H3V=CH2COZ+R1H         9.6E13      0.          0.        !(67,-
67)<TSAnG86>!
B1O+C2H4Z=R4CH3+R5CHO           8.1E6       1.88    0.2E3         !(68,-
68)<BAULCH94>!
B1O+C2H4Z=HCHO+B5CH2            4.00E5      1.88    0.2E3         !(69,-
69)<BAULCH94>!
B1O+C2H4Z=CH2COZ+H2             6.6E5       1.88    0.2E3         !(70,-
70)<BAULCH94>!
B1O+C2H4Z=R13CH2CHO+R1H         4.7E6       1.88    0.2E3         !(71,-
71)<BAULCH94>!
B1O+C2H4Z=R2OH+R10C2H3V         1.5E7       1.91    3.7E3         !(72,-
72)<MAHMUD87nIST>!
B1O+R11C2H5=HCHO+R4CH3          1.1E13      0.          0.        !(73,-
73)<BAULCH94>!
B1O+R11C2H5=CH3CHO+R1H          5.5e13      0.          0.        !(74,-
74)<BAULCH94>!
B1O+R11C2H5=C2H4Z+R2OH          3.0E13      0.          0.        !(75,-
75)<DAGAUT91>!
B1O+C2H6=R11C2H5+R2OH           1.0E9       1.5     5.8E3         !(76,-
76)<BAULCH94>!

!****** REACTIONS DE R2OH ******!
R1H+B1O+M=R2OH+M                1.18E19    -1.0       0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R1H+R2OH+M=H2O+M                 5.53E+22   -2.0         0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/
!      N2/0.4/ HE/0.35/
R2OH+H2=R1H+H2O                 1.0E8       1.6     3.3E3         !(79,-
79)<BAULCH94>!
R2OH+B3C=B2CO+R1H              5.0E13      0.          0.        !(80,-
80)<RAnZI94>!
R2OH+B4CH=R5CHO+R1H             3.0E13      0.          0.        !(81,-
81)<DAGAUT91>!
R2OH+B6CH2=HCHO+R1H             3.0E13      0.          0.        !(82,-
82)<TSAnG86>!
R2OH+B5CH2=HCHO+R1H             1.8E13      0.          0.        !(83,-
83)<TSAnG86>!
R2OH+R4CH3=B6CH2+H2O            7.2E13      0.      2.7E3         !(84,-
84)<BAULCH94>!
R2OH+R4CH3(+M)=CH3OH(+M)        6.0E13      0.          0.        !(85,-
85)<BAULCH94>!
      LOW     /1.4E44     -8.2          0./
      TROE    /0.82      200.        1438./
R2OH+R4CH3=HCHO+H2              3.2E12     -0.53   10.8E3         !(86,-
86)<DAGAUT91>!
R2OH+R4CH3=R7CH3O+R1H           5.7E12     -0.23   13.9E3         !(87,-
87)<DAGAUT91>!
R2OH+CH4=R4CH3+H2O              1.6E7       1.83    2.7E3         !(88,-
88)<BAULCH94>!
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!R2OH+R9C2H=C2H2+B1O           1.8E13      0.          0.         !(89,-
89)<TSAnG86>!
R2OH+R9C2H=B5CH2+B2CO          1.8E13      0.          0.         !(90,-
90)<TSAnG86>!
R2OH+R9C2H=R12CHCOZ+R1H        2.0E13      0.          0.         !(91,-
91)<DAGAUT91>!
R2OH+C2H2=R9C2H+H2O            3.385E+07   2.0    14000.0         !(92,-
92)<KONNOV00>!
R2OH+C2H2=CH2COZ+R1H           1.100E+13   0.0     7170.0         !(93,-
93)<KONNOV00>!
R2OH+C2H2=R4CH3+B2CO           4.8E-4      4.      -2.0E3         !(94,-
94)<DAGAUT91>!
R2OH+R10C2H3V=C2H2+H2O         3.0E13      0.          0.         !(95,-
95)<TSAnG86>!
R2OH+R10C2H3V=CH3CHO           3.0E13      0.          0.         !(96,-
96)<TSAnG86>!
R2OH+C2H4Z=R10C2H3V+H2O        2.0E13      0.       5.9E3         !(97,-
97)<BAULCH94>!
R2OH+C2H4Z=R4CH3+HCHO          2.0E12      0.       0.9E3         !(98,-
98)<GLARBORG86>!
R2OH+R11C2H5=C2H4Z+H2O         2.4E13      0.          0.         !(99,-
99)<TSAnG86>!
R2OH+R11C2H5=>R4CH3+R1H+HCHO   2.4E13      0.          0.         !(100)
<TSAnG86>!
R2OH+C2H6=R11C2H5+H2O          7.2E6       2.       0.9E3         !(101,-
101)<BAULCH94>!
R2OH+R2OH=H2O+B1O              1.5E9       1.14     0.1E3         !(102,-
102)<BAULCH94>!

!****** REACTIONS DE H2O ******!
H2O+B4CH=R6CH2OH               5.7E12      0.      -0.8E3         !(103,-
103)<BAULCH94>!
H2O+B6CH2=CH3OH                1.8E13      0.          0.         !(104,-
104)<TSAnG86>!

!REACTIOnS DE B2CO!
B2CO+R4CH3(+M)=R14CH3CO(+M)    5.0E11      0.       6.9E3         !(105,-
105)<BAULCH94>!
       LOW    /1.1E14      0.      3.8E3/
       TROE   /0.5         1.0      1.0E8/
B2CO+B1O+M=CO2+M               1.54E15     0.0      3.0E3         !(106,-
106)<TSAnG86>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
B2CO+R2OH=CO2+R1H              6.3E6       1.5     -0.5E3         !(107,-
107)<BAULCH94>!

!REACTIOnS DE R5CHO!
R5CHO+M=R1H+B2CO+M             1.9E17     -1.      17.0E3         !(108,-
108)<WAnG97>!
       H2/2.0/ B2CO/1.5/ CO2/2.0/ H2O/6.0/
R5CHO+R1H=H2+B2CO              9.0E13      0.          0.         !(109,-
109)<BAULCH94>!
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R5CHO+R1H=B1O+B5CH2            4.0E13      0.    102.5E3        !(110,-
110)<TSUBOI81nIST>!
R5CHO+B6CH2=R4CH3+B2CO         1.8E13      0.         0.        !(111,-
111)<TSAnG86>!
R5CHO+B5CH2=R4CH3+B2CO         1.8E13      0.         0.        !(112,-
112)<TSAnG86>!
R5CHO+R4CH3=CH4+B2CO           1.2E14      0.         0.        !(113,-
113)<TSAnG86>!
R5CHO+R4CH3=CH3CHO             1.8E13      0.         0.        !(114,-
114)<TSAnG86>!
R4CH3+HCHO=R5CHO+CH4           7.7E-8      6.1    1.97E3        !(115,-
115)<BAULCH94>!
R5CHO+R9C2H=C2H2+B2CO          6.0E13      0.         0.        !(116,-
116)<TSAnG86>!
R5CHO+R10C2H3V=C2H4Z+B2CO      9.0E13      0.         0.        !(117,-
117)<TSAnG86>!
R10C2H3V+HCHO=R5CHO+C2H4Z      5.4E3       2.81    5.9E3        !(118,-
118)<TSAnG86>!
R5CHO+R11C2H5=C2H6+B2CO        1.2E14      0.         0.        !(119,-
119)<TSAnG86>!
R11C2H5+HCHO=R5CHO+C2H6        5.57E3      2.81   5.86E3        !(120,-
120)<TSAnG86>!
R5CHO+B1O=R1H+CO2              3.0E13      0.         0.        !(121,-
121)<BAULCH94>!
R5CHO+B1O=R2OH+B2CO            3.0E13      0.         0.        !(122,-
122)<BAULCH94>!
R5CHO+R2OH=H2O+B2CO            1.1E14      0.         0.        !(123,-
123)<BAULCH94>!
R5CHO+R5CHO=HCHO+B2CO          3.0E13      0.         0.        !(124,-
124)<BAULCH94>!

!****** REACTIONS DE HCHO ******!
HCHO+M=R5CHO+R1H+M             1.40E36    -5.54   96.8E3        !(125,-
125)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+M=H2+B2CO+M               3.26E36    -5.54   96.8E3        !(126,-
126)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+R1H=R5CHO+H2              1.3E8       1.62    2.1E3        !(127,-
127)<BAULCH94>!
HCHO+B4CH=R13CH2CHO            9.6E13      0.     -0.5E3        !(128,-
128)<BAULCH94average>!
HCHO+B6CH2=R4CH3+R5CHO         1.2E12      0.         0.        !(129,-
129)<TSAnG86>!
HCHO+B1O=R5CHO+R2OH            4.1E11      0.57    2.7E3        !(130,-
130)<BAULCH94>!
HCHO+R2OH=R5CHO+H2O            7.82E07     1.63  -1.06E3        !MF
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!****** REACTIONS DE R7CH3O ******!
R7CH3O+M=HCHO+R1H+M             1.55E14     0.00   13.5E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
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!      N2/0.4/ HE/0.35/
R7CH3O+R1H=HCHO+H2              1.8E13      0.          0.         !(133,-
133)<BAULCH94>!
R7CH3O+B6CH2=R4CH3+HCHO         1.8E13      0.          0.         !(134,-
134)<TSAnG86>!
R7CH3O+B5CH2=R4CH3+HCHO         1.8E13      0.          0.         !(135,-
135)<TSAnG86>!
R7CH3O+R4CH3=HCHO+CH4           2.4E13      0.          0.         !(136,-
136)<TSAnG86>!
R7CH3O+CH4=R4CH3+CH3OH          1.6E11      0.       8.8E3         !(137,-
137)<TSAnG86>!
R7CH3O+R9C2H=HCHO+C2H2          2.4E13      0.          0.         !(138,-
138)<TSAnG86>!
R7CH3O+R10C2H3V=HCHO+C2H4Z      2.4E13      0.          0.         !(139,-
139)<TSAnG86>!
R7CH3O+C2H4Z=HCHO+R11C2H5       1.2E11      0.       6.7E3         !(140,-
140)<TSAnG86>!
R7CH3O+R11C2H5=HCHO+C2H6        2.4E13      0.          0.         !(141,-
141)<TSAnG86>!
R7CH3O+C2H6=R11C2H5+CH3OH       2.4E11      0.       7.0E3         !(142,-
142)<TSAnG86>!
R7CH3O+B1O=HCHO+R2OH            1.8E12      0.          0.         !(143,-
143)<BAULCH94>!
R7CH3O+R2OH=HCHO+H2O            1.8E13      0.          0.         !(144,-
144)<TSAnG86>!
R7CH3O+B2CO=R4CH3+CO2           1.6E13      0.      11.7E3         !(145,-
145)<TSAnG86>!
R7CH3O+R5CHO=CH3OH+B2CO         9.1E13      0.          0.         !(146,-
146)<TSAnG86>!
R7CH3O+HCHO=CH3OH+R5CHO         1.0E11      0.       3.0E3         !(147,-
147)<TSAnG86>!
R7CH3O+R7CH3O=CH3OH+HCHO        6.0E13      0.          0.         !(148,-
148)<TSAnG86>!


!****** REACTIONS DE R6CH2OH ******!
R6CH2OH+M=HCHO+R1H+M            1.26E16     0.00   30.0E3         !(149,-
149)<BAULCHLEEDS>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R6CH2OH+R1H=R4CH3+R2OH          9.6E13      0.          0.         !(150,-
150)<TSAnG87>!
R6CH2OH+R1H=HCHO+H2             6.0E12      0.          0.         !(151,-
151)<TSAnG87>!
R6CH2OH+H2=CH3OH+R1H            6.7E5       2.      13.4E3         !(152,-
152)<TSAnG87>!
R6CH2OH+B6CH2=CH3CHO+R1H        1.8E13      0.          0.         !(153,-
153)<TSAnG87>!
R6CH2OH+B5CH2=C2H4Z+R2OH        2.4E13      0.          0.         !(154,-
154)<TSAnG87>!
R6CH2OH+B5CH2=R4CH3+HCHO        1.2E12      0.          0.         !(155,-
155)<TSAnG87>!
R6CH2OH+R4CH3=C2H5OH           1.2E13      0.          0.         !(156,-
156)<TSAnG87>!
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R6CH2OH+R4CH3=CH4+HCHO          2.4E12      0.          0.         !(157,-
157)<TSAnG87>!
R6CH2OH+CH4=CH3OH+R4CH3         21.7        3.1    16.2E3          !(158,-
158)<TSAnG87>!
R6CH2OH+R9C2H=C2H2+HCHO         4.8E13      0.          0.         !(159,-
159)<TSAnG87>!
!la constante de vitesse du processus 159 est globalisee!
!R6CH2OH+R9C2H=C3H3+R2OH        1.2E13      0.          0.         !(159a,-
159a)<TSAnG87>!
!R6CH2OH+R9C2H=C2H2+HCHO        3.6E13      0.          0.         !(159b,-
159b)<TSAnG87>!
R6CH2OH+C2H2=R10C2H3V+HCHO      7.2E11      0.      9.0E3          !(160,-
160)<TSAnG87>!
R6CH2OH+R10C2H3V=C2H4Z+HCHO     4.2E13      0.          0.         !(161,-
161)<TSAnG87>!
!La constante de vitesse  du processus 161 est globalisee!
R6CH2OH+R11C2H5=C2H4Z+CH3OH     2.4E12      0.          0.         !(162,-
162)<TSAnG87>!
R6CH2OH+R11C2H5=C2H6+HCHO       2.4E12      0.          0.         !(163,-
163)<TSAnG87>!
R6CH2OH+C2H6=CH3OH+R11C2H5      199.        3.     14.0E3          !(164,-
164)<TSAnG87>!
R6CH2OH+B1O=HCHO+R2OH           4.2E13      0.          0.         !(165,-
165)<TSAnG87>!
R6CH2OH+R2OH=H2O+HCHO           2.4E13      0.          0.         !(166,-
166)<TSAnG87>!
!attention (167) metatheses dans les reactions de CH3OH!
!R6CH2OH+H2O=CH3OH+R2OH         1.6E14      0.     26.3E3          !(167,-
167)<TSUBOI81nIST>!
R6CH2OH+R5CHO=CH3OH+B2CO        1.2E14      0.          0.         !(168,-
168)<TSAnG87>!
R6CH2OH+R5CHO=HCHO+HCHO         1.8E14      0.          0.         !(169,-
169)<TSAnG87>!
R6CH2OH+HCHO=CH3OH+R5CHO        5.5E3       2.8     5.9E3          !(170,-
170)<TSAnG87>!
R6CH2OH+R7CH3O=CH3OH+HCHO       2.4E13      0.          0.         !(171,-
171)<TSAnG87>!
R6CH2OH+R6CH2OH=CH3OH+HCHO      1.4E13      0.          0.         !(172,-
172)<TSAnG87>!
!la constante de vitesse du processus 172 est globalisee!
!R6CH2OH+R6CH2OH=CH3OH+HCHO     4.8E12      0.          0.         !(172a,-
172a)<TSAnG87>!
!R6CH2OH+R6CH2OH=HOCH2CH2OH     9.6E12      0.          0.         !(172b,-
172b)<TSAnG87>!

!****** REACTIONS DE CH3OH ******!
CH3OH+R1H=R4CH3+H2O             2.0E14      0.      5.3E3          !(173,-
173)<HIDAKA89nIST>!
CH3OH+R1H=R7CH3O+H2             4.2E6       2.1     4.9E3          !(174,-
174)<TSAnG87>!
CH3OH+B6CH2=R6CH2OH+R4CH3       1.5E12      0.          0.         !(175,-
175)<TSAnG87>!
CH3OH+B5CH2=R4CH3+R6CH2OH       31.9        3.2     7.2E3          !(176,-
176)<TSAnG87>!
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CH3OH+B5CH2=R4CH3+R7CH3O       14.4        3.1     6.9E3         !(177,-
177)<TSAnG87>!
CH3OH+R9C2H=C2H2+R6CH2OH       6.0E12      0.         0.         !(178,-
178)<TSAnG87>!
CH3OH+R9C2H=C2H2+R7CH3O        1.2E12      0.         0.         !(179,-
179)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R6CH2OH   31.9        3.2     7.2E3         !(180,-
180)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R7CH3O    14.4        3.1     6.9E3         !(181,-
181)<TSAnG87>!
CH3OH+B1O=R6CH2OH+R2OH         3.4E13      0.      5.5E3          !(182,-
182)<GROTHEER81nIST>!
CH3OH+B1O=R7CH3O+R2OH          1.0E13      0.      4.7E3         !(183,-
183)<WARnATZ84>!
!modification des metatheses avec OH!
!CH3OH+R2OH=R7CH3O+H2O         1.0E13      0.      1.7E3         !(184,-
184)<WARnATZ84>!
CH3OH+R2OH=R6CH2OH+H2O         3.1E06      2.     -3.4E2         !(184a,-
184a)<Atkinson86>85%!
CH3OH+R2OH=R7CH3O+H2O          5.4E05      2.     -3.4E2         !(184b,-
184b)<Atkinson86>15%!
CH3OH+R7CH3O=CH3OH+R6CH2OH     3.0E11      0.      4.1E3         !(185,-
185)<TSAnG87>!

!****** REACTIONS DE R12CHCOD ******!
R12CHCOZ+M=B4CH+B2CO+M          6.0E15      0.     58.8E3         !(186,-
186)<DAGAUT91>!
R12CHCOZ+R1H=B5CH2+B2CO         1.5E14      0.         0.         !(187a,-
187a)<BAULCH94>!
R12CHCOZ+R1H=B6CH2+B2CO         1.3E14      0.         0.         !(187b,-
187b)<PEETERS97>!
R12CHCOZ+B5CH2=R9C2H+HCHO       1.0E13      0.      2.0E3         !(188,-
188)<DAGAUT91>!
R12CHCOZ+B5CH2=R10C2H3V+B2CO    3.0E13      0.         0.         !(189,-
189)<DAGAUT91>!
R12CHCOZ+B1O=>B2CO+B2CO+R1H     9.6E13      0.         0.         !
(190)<BAULCH94>!
R12CHCOZ+R2OH=>R5CHO+B2CO+R1H   1.0E13      0.         0.         !
(191)<DAGAUT91>!


!****** REACTIONS DE CH2COD ******!
CH2COZ+M=B6CH2+B2CO+M           6.57E15     0.0    57.6E3         !(192,-
192)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
CH2COZ+M=R12CHCOZ+R1H+M         2.7E17      0.     87.0E3         !(193,-
193)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
CH2COZ+R1H=R4CH3+B2CO           1.8E13      0.      3.4E3         !(194,-
194)<BAULCH94>!
CH2COZ+R1H=R12CHCOZ+H2          5.0E13      0.      8.0E3         !(195,-
195)<DAGAUT91>!
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CH2COZ+B5CH2=C2H4Z+B2CO        1.3E14      0.         0.        !(196,-
196)<CAnOSA-MAS84nIST>!
CH2COZ+B1O=B5CH2+CO2           1.8E12      0.      1.3E3        !(197,-
197)<DAGAUT91>!
CH2COZ+B1O=R12CHCOZ+R2OH       1.0E13      0.      8.0E3        !(198,-
198)<DAGAUT91>!
CH2COZ+R2OH=R12CHCOZ+H2O       7.5E12      0.      2.0E3        !(199,-
199)<DAGAUT91>!
!CH2COZ+R2OH=R5CHO+HCHO        2.8E13      0.        0.         !(200,-
200)<VAnDOOREn77nIST>!
CH2COZ+R2OH=R4CH3+CO2          2.52E12     0.         0.        !(200a,-
200a)<BAULCH LEEDS>!
CH2COZ+R2OH=R6CH2OH+B2CO       4.68E12     0.         0.        !(200b,-
200b)<BAULCH LEEDS>!


!****** REACTIONS DE R14CH3CO ******!
R14CH3CO+R1H=R4CH3+R5CHO        9.6E13      0.         0.        !(201,-
201)<TSAnG86>!
R14CH3CO+B6CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(202,-
202)<TSAnG86>!
R14CH3CO+B5CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(203,-
203)<TSAnG86>!
R14CH3CO+B1O=R4CH3+CO2          9.6E12      0.         0.        !(204,-
204)<TSAnG86>!
R14CH3CO+R2OH=CH2COZ+H2O        1.2E13      0.         0.        !(205,-
205)<TSAnG86>!
R14CH3CO+R2OH=>R4CH3+B2CO+R2OH  3.0E13      0.         0.        !
(206)<TSAnG86>!
R14CH3CO+R5CHO=CH3CHO+B2CO      9.0E12      0.         0.        !(207,-
207)<TSAnG86>!
R14CH3CO+HCHO=CH3CHO+R5CHO      1.8E11      0.      12.9E3       !(208,-
208)<TSAnG86>!
R14CH3CO+R7CH3O=CH3OH+CH2COZ    6.0E12      0.         0.        !(209,-
209)<TSAnG86>!
R14CH3CO+R7CH3O=HCHO+CH3CHO     6.0E12      0.         0.        !(210,-
210)<TSAnG86>!
R14CH3CO+CH3OH=CH3CHO+R6CH2OH   4.85E3      3.      12.3E3       !(211,-
211)<TSAnG87>!
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 1.2E13      0.         0.        !(212,-
212)<TSAnG86>!

!****** REACTIONS DE R13CH2CHO ******!
!R13CH2CHO=R14CH3CO               1.0E13      0.      47.0E3          !
(213,-213)<COLKET75nIST>!
!R13CH2CHO=R1H+CH2COZ             1.6E13      0.      35.0E3          !
(214,-214)<COLKET75nIST>!
R13CH2CHO=R4CH3+B2CO                2.93E12     0.29    40.3E3!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.
R13CH2CHO=R1H+CH2COZ                1.43E15     -0.15   45.6E3 !at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.


!****** REACTIONS DE CH3CHO ******!
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!CH3CHO+R1H=H2+R14CH3CO           4.0E13      0.       4.2E3          !
(215,-215)<WARnATZ84>!
!CH3CHO+R4CH3=R14CH3CO+CH4        2.0E-6      5.6      2.5E3          !
(216,-216)<BAULCH94>!
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO   8.1E10      0.       3.7E3          !
(217,-217)<SCHERZER87>!
!CH3CHO+R11C2H5=C2H6+R14CH3CO     1.3E12      0.       8.5E3          !
(218,-218)<HOHLEIn70>!
!CH3CHO+B1O=R14CH3CO+R2OH         1.4E13      0.       2.3E3          !
(219,-219)<CAVAnAGH90>!
!CH3CHO+R2OH=R14CH3CO+H2O         4.2E12      0.       0.5E3          !
(220,-220)<CAVAnAGH90>!
!CH3CHO+R7CH3O=R14CH3CO+CH3OH     2.4E11      0.       1.8E3          !
(221,-221)<CAVAnAGH90>!
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 2.5E7       0.         0.           !
(222,-222)<SCHUCHMAnn70nIST>!

!****** REACTIONS DE C2H4O# ******!
C2H4O#3=CH4+B2CO                   1.2E13      0.      57.2E3   !(223,-
223)<LIFSHITZ83nIST>!
C2H4O#3=CH3CHO                     7.3E13      0.      57.2E3   !(224,-
224)<LIFSHITZ83nIST>!
C2H4O#3=R4CH3+R5CHO                3.6E13      0.      57.2E3   !(225,-
225)<LIFSHITZ83nIST>!
C2H4O#3+R1H=H2+R13CH2CHO           2.0E13      0.       8.3E3   !(226,-
226)<LIFSHITZ83nIST*>!
C2H4O#3+R1H=H2O+R10C2H3V           5.0E9       0.       5.0E3   !(227,-
227)<LIFSHITZ83nIST>!
C2H4O#3+R1H=C2H4Z+R2OH             9.5E10      0.       5.0E3   !(228,-
228)<LIFSHITZ83nIST>!
C2H4O#3+R4CH3=CH4+R13CH2CHO        1.1E12      0.      11.8E3   !(229,-
229)<BALDWIn84nIST*>!
C2H4O#3+R4CH3=R11C2H5+HCHO         1.4E11      0.       7.6E3   !(230,-
230)<RAnZI94>!
C2H4O#3+R4CH3=C2H4Z+R7CH3O         1.5E10      0.       7.6E3   !(231,-
231)<RAnZI94>!
C2H4O#3+R9C2H=C2H2+R13CH2CHO       1.2E12      0.       9.8E3   !(232,-
232)<RAnZI94>!
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO   2.0E12      0.       9.3E3   !(233,-
233)<RAnZI94>!
C2H4O#3+R11C2H5=C2H6+R13CH2CHO     6.8E11      0.      11.4E3   !(234,-
234)<RAnZI94>!
C2H4O#3+B1O=R2OH+R13CH2CHO         1.9E12      0.       5.2E3   !(235,-
235)<BOGAn78nIST>!
C2H4O#3+R2OH=H2O+R13CH2CHO         1.8E13      0.       3.6E3   !(236,-
236)<BALDWIn84nIST*>!
C2H4O#3+R5CHO=HCHO+R13CH2CHO       3.7E12      0.      15.8E3   !(237,-
237)<RAnZI94>!
C2H4O#3+R7CH3O=CH3OH+R13CH2CHO     1.3E12      0.       5.8E3   !(238,-
238)<RAnZI94>!
C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO    8.4E11      0.      13.4E3   !(239,-
239)<RAnZI94>!
C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO  4.0E12      0.      17.5E3   !(240,-
240)<RAnZI94>!
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C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO 6.8E11      0.      15.4E3    !(241,-
241)<RAnZI94>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!

!****** REACTIONS DE R15C2H5O ******!

!****** REACTIONS DE C2H5OH ******!

!Voir Plus bas meca 10a Luc Sy Tran

!****** REACTIONS DE O2 ******!
B1O+B1O+M=O2+M                 5.40E13     0.   -1.79E3    !(244,-
244)<BAULCH94>!
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!       N2/0.4/ HE/0.35/
O2+R1H=R2OH+B1O                9.8E13      0.     14.8E3   !(245,-
245)<BAULCH94>!
!O2+R1H+M=R3OOH+M              2.10E18    -0.8    0.00     !(246,-
246)<baseLeeds>!
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H+H2O=R3OOH+H2O           6.90E15    0.0    -2.10E3   !(246,-
246bis)<base Leeds>!

O2+R1H(+M)=R3OOH(+M)           4.52E13     0.       0.          !(246,-
246)<COBOS85>!
               LOW   /1.8E18     -0.8       0.00/                    !k0
BAULCH94!
               TROE  /0.5         1.0      1.0E8/
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H(+H2O)=R3OOH(+H2O)      1.63E14     0.       761.   !(246b,-
246b)<COBOS85>!
O2+R1H(+H2O)=R3OOH(+H2O)       4.52E13     0.         0.   !(246b,-
246b)<BAULCH94>!
               LOW   /6.9E15     0.0      -2080/
               TROE  /0.45       1.0      1.0E8/
O2+B3C=B2CO+B1O               1.2E14      0.         0.    !(247,-
247)<RAnZI94>!
O2+B4CH=R5CHO+B1O              3.3E13      0.         0.   !(248,-
248)<DAGAUT91>!
O2+B4CH=B2CO+R2OH              3.2E13      0.         0.   !(249,-
249)<PEETERS97>!
O2+B6CH2=>B2CO+R2OH+R1H        3.1E12      0.         0.   !
(250)<BAULCH94>!
O2+B5CH2=R5CHO+R2OH            4.3E10      0.     -0.5E3   !(251,-
251)<DAGAUT91>!
O2+B5CH2=CO2+H2                6.9E11      0.      0.5E3   !(252,-
252)<DAGAUT91>!
O2+B5CH2=>CO2+R1H+R1H          1.6E12      0.      1.0E3   !
(253)<DAGAUT91>!
O2+B5CH2=B2CO+H2O              1.9E10      0.     -1.0E3   !(254,-
254)<DAGAUT91>!
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O2+B5CH2=>B2CO+R2OH+R1H          8.6E10      0.      -0.5E3   !
(255)<DAGAUT91>!
O2+B5CH2=HCHO+B1O                1.0E14      0.       4.5E3   !(256,-
256)<DAGAUT91>!
O2+R4CH3(+M)=R8CH3OO(+M)         7.8E8       1.2         0.   !(257,-
257)<BAULCH94>!
                    LOW   /5.6E25     -3.3        0./
                    TROE  /0.36        1.0      1.0E8/
O2+R4CH3=R7CH3O+B1O              1.3E14      0.      31.3E3   !(258,-
258)<BAULCH94>!
!O2+R4CH3=R7CH3O+B1O             1.6E13      0.      31.4E3   !(258,-
258)<HWAnG&RABInOVITCH99>!

O2+R4CH3=HCHO+R2OH               3.0E30     -4.69    36.6E3   !(259,-
259)<DAGAUT91>!
O2+CH4=R4CH3+R3OOH               4.0E13      0.      56.7E3   !(260,-
260)<BAULCH94>!
O2+R9C2H=B2CO+R5CHO              3.8E13     -0.16        0.   !(261,-
261)<TIESEMAnn97/TSAnG86>!
O2+R9C2H=R12CHCOZ+B1O            9.0E12     -0.16        0.   !(262,-
262)<TIESEMAnn97/TSAnG86>!
O2+C2H2=R9C2H+R3OOH              1.2E13      0.      74.5E3   !(263,-
263)<TSAnG86>!
!O2+C2H2=R12CHCOZ+R2OH           2.0E8       1.5     30.1E3   !(264,-
264)<DAGAUT91>!
O2+C2H2=R5CHO+R5CHO              7.0E7       1.8     30.6E3   !(264,-
264)<BEnSOn95>!

!O2+R10C2H3V=C2H2+R3OOH          1.2E11      0.          0.   !(265,-
265)<TSAnG86>!

!O2+R10C2H3V=C2H2+R3OOH          1.6E14     -0.83     2.5E3   !(265,-
265)<WAnG97>!
!at 760 Torr
!O2+R10C2H3V=HCHO+R5CHO          8.6E21     -2.97     3.3E3   !(266a,-
266a)<WAnG97>!
!O2+R10C2H3V=B1O+R13CH2CHO       1.2E13     -0.12     1.7E3   !(266b,-
266b)<WAnG97>!
!at 20-90 Torr
!O2+R10C2H3V=HCHO+R5CHO          1.6E21     -2.78     2.5E3   !(266a,-
266a)<WAnG97>!
!O2+R10C2H3V=B1O+R13CH2CHO       2.5E12      0.057    0.9E3   !(266b,-
266b)<WAnG97>!

O2+R10C2H3V=C2H2+R3OOH           1.34E6      1.61    -0.4E3   !(265,-
265)<MEBEL nIST>!
O2+R10C2H3V=HCHO+R5CHO           4.5E16     -1.39     1.0E3   !(266a,-
266a)<MEBEL nIST>!
O2+R10C2H3V=B1O+R13CH2CHO        3.3E11     -0.29       10.   !(266b,-
266b)<MEBEL nIST>!

O2+C2H4Z=R10C2H3V+R3OOH          4.2E13      0.      57.4E3   !(267,-
267)<TSAnG86>!
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O2+R11C2H5=R17C2H5OO          2.2E10      0.77    -0.6E3    !(268,-
268)<WAGnER90>!
O2+R11C2H5=C2H4Z+R3OOH         8.4E11      0.       3.9E3    !(269,-
269)<TSAnG86>!
O2+R11C2H5=R15C2H5O+B1O        1.2E13     -0.2     27.9E3    !(270,-
270)<BOZZELLI90nIST>!
O2+R11C2H5=CH3CHO+R2OH         6.0E10      0.       6.9E3    !(271,-
271)<TSAnG86>!
O2+C2H6=R11C2H5+R3OOH          6.0E13      0.      51.7E3    !(272,-
272)<BAULCH94>!
O2+R2OH=R3OOH+B1O              2.2E13      0.      52.5E3    !(273,-
273)<TSAnG86>!
O2+B2CO=CO2+B1O                2.5E12      0.      47.7E3    !(274,-
274)<TSAnG86>!
!O2+R5CHO=B2CO+R3OOH           5.1E13      0.       1.7E3    !(275,-
275)<TSAnG86>!
O2+R5CHO=B2CO+R3OOH            7.6E12      0.      0.41E3    !(275,-
275)<TIMOnEn88>!
O2+HCHO=R5CHO+R3OOH            2.0E13      0.      38.8E3    !(276,-
276)<TSAnG86)!
O2+R7CH3O=HCHO+R3OOH           2.2E10      0.       1.7E3    !(277,-
277)<BAULCH94>!
O2+R6CH2OH=HCHO+R3OOH          1.2E12      0.          0.    !(278,-
278)<TSAnG87>!
O2+CH3OH=R6CH2OH+R3OOH         2.0E13      0.      44.9E3    !(279,-
279)<TSAnG87>!
O2+R12CHCOZ=>B2CO+B2CO+R2OH    1.5E12      0.       2.5E3    !(280)
<DAGAUT91>!
!O2+CH2COZ=HCHO+CO2            1.0E8       0.          0.    !(281,-
281)<DAGAUT91>!bizarre
O2+R14CH3CO=R18CH3COOO        2.4E12      0.          0.     !(282,-
282)<COX90>!
O2+R13CH2CHO=>HCHO+R2OH+B2CO   5.9E9       0.      -1.4E3    !(283)
<COX90>!
O2+R13CH2CHO=CH2COZ+R3OOH      1.0E10      0.      -1.4E3    !(284,-
284)<COX90>!
O2+CH3CHO=R14CH3CO+R3OOH       5.0E13      0.      36.4E3    !(285,-
285)<COX90>!
! ajout demande par Laetitia le 25 Avril 95
O2+CH3CHO=R13CH2CHO+R3OOH      1.0E13      0.5     46.0E3    !(285',-
285)<Ranzi94>!
O2+C2H4O#3=R3OOH+R13CH2CHO     5.0E13      0.      48.0E3    !(286,-
286)<RAnZI94>!
!O2+R15C2H5O=CH3CHO+R3OOH       6.0E10      0.       1.7E3  !(287,-
287)<BAULCH94>!

!****** REACTIONS DE R3OOH ******!
R3OOH+R1H=H2+O2                 4.3E13      0.       1.4E3  !(288,-
288)<BAULCH94>!
R3OOH+R1H=2R2OH                 1.7E14      0.       0.9E3  !(289,-
289)<BAULCH94>!
R3OOH+R1H=H2O+B1O               3.0E13      0.       1.7E3  !(290,-
290)<BAULCH94>!
```

```
R3OOH+B6CH2=HCHO+R2OH           3.0E13      0.          0.  !(291,-
291)<TSAnG86>!
R3OOH+B5CH2=HCHO+R2OH           1.8E13      0.          0.  !(292,-
292)<TSAnG86>!
R3OOH+R4CH3=R7CH3O+R2OH         1.8E13      0.          0.  !(293,-
293)<BAULCH94>!
!R3OOH+R4CH3=R7CH3O+R2OH        4.0E13      0.       5.0E3  !(293,-
293)<DAGAUT>
R3OOH+CH4=R4CH3+H2O2            9.0E12      0.      24.6E3  !(294,-
294)<BAULCH94>!
R3OOH+R9C2H=R12CHCOZ+R2OH       1.8E13      0.          0.  !(295,-
295)<TSAnG86>!
R3OOH+C2H2=CH2COZ+R2OH          6.0E9       0.       8.0E3  !(296,-
296)<TSAnG86>!
!incertitude au moins un facteur 10
R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO 3.0E13      0.          0.  !(297)
<TSAnG86>!
R3OOH+C2H4Z=CH3CHO+R2OH         6.0E9       0.       7.9E3  !(298,-
298)<TSAnG86>!
R3OOH+C2H4Z=C2H4O#3+R2OH        2.2E12      0.      17.2E3  !(299,-
299)<BAULCH94>!
R3OOH+R11C2H5=>R4CH3+HCHO+R2OH  2.4E13      0.          0.  !(300)
<TSAnG86>!
R3OOH+R11C2H5=C2H4Z+H2O2        3.0E11      0.          0.  !(301,-
301)<TSAnG86>!
R3OOH+C2H6=R11C2H5+H2O2         1.3E13      0.      20.4E3  !(302,-
302)<BAULCH94>!
R3OOH+R2OH=H2O+O2               2.9E13      0.      -0.5E3  !(303,-
303)<BAULCH94>!
R3OOH+B2CO=CO2+R2OH             1.57E05     2.18    17.9E3  !MF Wang, J.
Phys. Chem. A 111(2007)4031 - 4042
R3OOH+R5CHO=>R2OH+R1H+CO2       3.0E13      0.          0.  !(305)
<TSAnG86>!
R3OOH+HCHO=R5CHO+H2O2           3.0E12      0.      13.0E3  !(306,-
306)<BAULCH94>!
R3OOH+R7CH3O=HCHO+H2O2          3.0E11      0.          0.  !(307,-
307)<TSAnG86>!
R3OOH+R6CH2OH=HCHO+H2O2         1.2E13      0.          0.  !(308,-
308)<TSAnG87>!
R3OOH+CH3OH=R6CH2OH+H2O2        9.6E10      0.      12.6E3  !(309,-
309)<TSAnG87>!
R3OOH+R14CH3CO=>R4CH3+CO2+R2OH  3.0E13      0.          0.  !
(310)<TSAnG86>!
R3OOH+CH3CHO=R14CH3CO+H2O2      1.0E12      0.      10.0E3  !(311,-
311)<CAVAnAGH90>!
R3OOH+C2H4O#3=H2O2+R13CH2CHO    1.6E12      0.      15.0E3  !(312,-
312)<RAnZI94>
R3OOH+R3OOH=H2O2+O2             1.3E11      0.     -1.63E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE
R3OOH+R3OOH=H2O2+O2             4.2E14      0.     11.98E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE
```

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!****** REACTIONS DE H2O2 ******!
!R2OH+R2OH(+ M)=>H2O2 (+ M)     7.23E13    -0.37    0.00
!       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /5.53E19  -0.76     0.00 /
!        TROE /0.5 1 1.E8/
!H2O2(+M)=>R2OH+R2OH(+M)        3.00E14     0.00    48.5E3
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /3.0E17   0.0     45.5E3/
!       TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601
H2O2(+M)=R2OH+R2OH(+M)        1.99E12     0.9    4.8749E4 !<BAULCH94>!
          AR/0.68/ O2/0.79/ N2/1.00/ CO2/1.06/ H2O/5.1/ H2O2/5.2/
        LOW  /3.65e24   -2.3   4.8749E4/
        TROE /0.43 1 1.E8/

H2O2+R1H=H2+R3OOH              1.7E12      0.      3.7E3   !(315,-
315)<BAULCH94>!
H2O2+R1H=H2O+R2OH              1.0E13      0.      3.6E3   !(316,-
316)<BAULCH94>!
H2O2+B6CH2=R7CH3O+R2OH         3.0E13      0.         0.   !(317,-
317)<TSAnG86>!
H2O2+R10C2H3V=C2H4Z+R3OOH      1.2E10      0.     -0.6E3   !(318,-
318)<TSAnG86>!
H2O2+B1O=R2OH+R3OOH            6.6E11      0.      4.0E3   !(319,-
319)<BAULCH94>!
H2O2+R2OH=H2O+R3OOH            7.8E12      0.      1.3E3   !(320,-
320)<BAULCH94>!

!****** REACTIONS DE CO2 ******!
CO2+B5CH2=HCHO+B2CO            2.3E10      0.         0.   !(321,-
321)<TSAnG86>!

!****** REACTIONS DE R8CH3OO ******!
R8CH3OO=HCHO+R2OH                1.5E13      0.     47.0E3 !(322,-
322)<RAnZI94>!
R8CH3OO+R1H=R7CH3O+R2OH          9.6E13      0.         0. !(323,-
323)<TSAnG86>!
R8CH3OO+H2=CH3OOH+R1H            3.0E13      0.     26.0E3 !(324,-
324)<TSAnG86>!
R8CH3OO+B6CH2=HCHO+R7CH3O        1.8E13      0.         0. !(325,-
325)<TSAnG86>!
R8CH3OO+B5CH2=HCHO+R7CH3O        1.8E13      0.         0. !(326,-
326)<TSAnG86>!
R8CH3OO+R4CH3=R7CH3O+R7CH3O      5.0E12      0.     -1.4E3 !(327,-
327)<CAVAnAGH90>!
R8CH3OO+CH4=CH3OOH+R4CH3         1.8E11      0.     18.5E3 !(328,-
328)<TSAnG86>!
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ    2.4E13      0.         0. !(329,-
329)<TSAnG86>!
!R8CH3OO+C2H2=CH3OOH+R9C2H        5.6E11      0.     24.5E3 !(330,-
330)<RAnZI94>! MF car i<<0
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R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 2.4E13      0.         0. !(331,-
331)<TSAnG86*>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3      1.1E15      0.     20.0E3 !(332,-
332)<nIKISHA81/MOSHKInA80nIST>!
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V     3.9E12      0.     24.5E3 !(333,-
333)<RAnZI94>!
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O   2.4E13      0.         0. !(334,-
334)<TSAnG86>!
R8CH3OO+C2H6=CH3OOH+R11C2H5       2.9E11      0.     14.9E3 !(335,-
335)<TSAnG86>!
R8CH3OO+B1O=R7CH3O+O2             3.6E13      0.         0. !(336,-
336)<TSAnG86>!
R8CH3OO+R2OH=CH3OH+O2             6.0E13      0.         0. !(337,-
337)<TSAnG86>!
R8CH3OO+R2OH=R7CH3O+R3OOH         3.0E12      0.         0. !(338,-
338)<RAnZI94>!
R8CH3OO+B2CO=R7CH3O+CO2           1.0E14      0.     24.0E3 !(339,-
339)<RAnZI94>!
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2     3.0E13      0.         0. !(340)
<TSAnG86>!
R8CH3OO+HCHO=CH3OOH+R5CHO         1.0E12      0.     12.1E3 !(341,-
341)<CAVAnAGH90>!
R8CH3OO+R7CH3O=HCHO+CH3OOH        3.0E11      0.         0. !(342,-
342)<TSAnG86>!
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO 1.2E13      0.         0. !
(343)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R6CH2OH      1.8E12      0.     13.7E3 !(344,-
344)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R7CH3O       2.8E11      0.     18.8E3 !(345,-
345)<RAnZI94>!
R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ    1.7E12      0.     27.0E3 !(346,-
346)<RAnZI94>!
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O 2.4E13      0.         0. !(347,-
347)<TSAnG86>!
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO    1.0E12      0.     12.1E3 !(348,-
348)<CAVAnAGH90>!
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO   1.7E12      0.     19.2E3 !(349,-
349)<RAnZI94>!
R8CH3OO+C2H4O#3=CH3OOH+R13CH2CHO  2.2E12      0.     16.0E3 !(350,-
350)<RAnZI94>!
R8CH3OO+R3OOH=CH3OOH+O2           2.5E11      0.     -1.6E3 !(351,-
351)<BAULCH94>!
R8CH3OO+R3OOH=>O2+HCHO+H2O        5.0E10      0.         0. !
(352)<RAnZI94>!
R8CH3OO+H2O2=CH3OOH+R3OOH         2.4E12      0.      9.9E3 !(353,-
353)<TSAnG86>!
R8CH3OO+R8CH3OO=CH3OH+HCHO+O2     2.5E10      0.     -0.8E3 !(354,-
354)<BAULCH94>!
R8CH3OO+R8CH3OO=R7CH3O+R7CH3O+O2  2.5E10      0.     -0.8E3 !(355,-
355)<BAULCH94>!

!****** REACTIOnS DE CH3OOH ******!
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CH3OOH=R7CH3O+R2OH                6.0E14      0.     42.3E3 !(356,-
356)<BAULCH94>!
CH3OOH+B1O=R8CH3OO+R2OH           2.0E13      0.      4.8E3 !(357,-
357)<BAULCH94average>!
CH3OOH+R2OH=H2O+R8CH3OO           1.8E12      0.    -0.37E3 !(358,-
358)<BAULCH94average>!
CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO    1.5E11      0.      6.5E3 !
(359)<RAnZI94>!

!****** REACTIOnS DE R17C2H5OO ******!
R17C2H5OO=R16C2H4OOH                4.2E12      0.     36.9E3 !(360,-
360)<HUGHES93>!
R17C2H5OO+H2=C2H5OOH+R1H            7.9E12      0.     21.0E3 !(361,-
361)<RAnZI94>!
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O     2.0E12      0.     -1.2E3 !(362,-
362)<RAnZI94>!
R17C2H5OO+CH4=C2H5OOH+R4CH3         3.9E12      0.     24.0E3 !(363,-
363)<RAnZI94>!
R17C2H5OO+C2H2=C2H5OOH+R9C2H        5.6E11      0.     24.4E3 !(364,-
364)<RAnZI94>!
R17C2H5OO+C2H4Z=C2H5OOH+R10C2H3V    3.9E12      0.     24.4E3 !(365,-
365)<RAnZI94>!
R17C2H5OO+C2H4Z=R15C2H5O+C2H4O#3    2.3E16      0.     21.9E3 !(366,-
366)<MOSHKInA80nIST>!
R17C2H5OO+C2H6=C2H5OOH+R11C2H5      5.1E12      0.     19.5E3 !(367,-
367)<RAnZI94>!
R17C2H5OO+H2O=C2H5OOH+R2OH          5.6E12      0.     30.6E3 !(368,-
368)<RAnZI94>!
R17C2H5OO+B2CO=CO2+R15C2H5O         1.0E14      0.     24.0E3 !(369,-
369)<RAnZI94>!
R17C2H5OO+HCHO=C2H5OOH+R5CHO        4.5E12      0.     14.4E3 !(370,-
370)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R7CH3O      2.8E11      0.     18.4E3 !(371,-
371)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R6CH2OH     2.8E12      0.     19.5E3 !(372,-
372)<RAnZI94>!
R17C2H5OO+CH2COZ=C2H5OOH+R12CHCOZ   1.7E12      0.     24.4E3 !(373,-
373)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R14CH3CO   3.9E12      0.     14.4E3 !(374,-
374)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R13CH2CHO  1.7E12      0.     19.5E3 !(375,-
375)<RAnZI94>!
R17C2H5OO+C2H4O#3=C2H5OOH+R13CH2CHO 2.2E12      0.     16.3E3 !(376,-
376)<RAnZI94>!
R17C2H5OO+R3OOH=O2+C2H5OOH          3.9E11      0.     -1.3E3 !(377,-
377)<BAULCH89>!
!Rate constant measured between 240 and 380K!
R17C2H5OO+H2O2=C2H5OOH+R3OOH        4.5E11      0.     10.8E3 !(378,-
378)<RAnZI94>!
R17C2H5OO+R8CH3OO=>R15C2H5O+R7CH3O+O2  2.0E11      0.         0. !
(379)<RAnZI94>!
R17C2H5OO+CH3OOH=C2H5OOH+R8CH3OO    1.1E12      0.     16.3E3 !(380,-
380)<RAnZI94>!
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R17C2H5OO+R17C2H5OO=2R15C2H5O+O2   4.1E10      0.      0.2E3 !(381,-
381)<LIGHTFOOT92>!
R17C2H5OO+R17C2H5OO=C2H5OH+CH3CHO+O2  1.8E10      0.       0.2E3 !(382,-
382)<LIGHTFOOT92>!

!****** REACTIONS DE R16C2H4OOH ******!
R16C2H4OOH=C2H4O#3+R2OH            1.5E11      0.     20.0E3 !(383,-
383)<RAnZI94>!
R16C2H4OOH=R6CH2OH+HCHO            2.5E13      0.     27.5E3 !(384,-
384)<RAnZI94>!
R16C2H4OOH=C2H4Z+R3OOH             2.0E13      0.     23.5E3 !(385,-
385)<RAnZI94>!

!****** REACTIONS DE C2H5OOH ******!
C2H5OOH=R15C2H5O+R2OH               4.0E15      0.     42.9E3 !(386,-
386)<BAULCH94>!
C2H5OOH+R1H=>CH3CHO+R2OH+H2         3.2E13      0.      7.7E3 !
(387)<RAnZI94>!
C2H5OOH+R4CH3=>CH3CHO+R2OH+CH4      5.7E11      0.      8.7E3 !
(388)<RAnZI94>!
C2H5OOH+R9C2H=>CH3CHO+R2OH+C2H2     6.0E11      0.      9.2E3 !
(389)<RAnZI94>!
C2H5OOH+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12      0.      8.7E3 !
(390)<RAnZI94>!
C2H5OOH+R11C2H5=>CH3CHO+R2OH+C2H6   3.4E11      0.     11.4E3 !
(391)<RAnZI94>!
C2H5OOH+R2OH=>CH3CHO+R2OH+H2O       5.9E12      0.      0.9E3 !
(392)<RAnZI94>!
C2H5OOH+R5CHO=>CH3CHO+R2OH+HCHO     1.8E12      0.     16.7E3 !
(393)<RAnZI94>!
C2H5OOH+R7CH3O=>CH3CHO+R2OH+CH3OH   6.3E11      0.      5.5E3 !
(394)<RAnZI94>!
C2H5OOH+R6CH2OH=>CH3CHO+R2OH+CH3OH  4.2E11      0.     13.6E3 !
(395)<RAnZI94>!
C2H5OOH+R14CH3CO=>2CH3CHO+R2OH      2.0E12      0.     18.5E3 !
(396)<RAnZI94>!
C2H5OOH+R13CH2CHO=>2CH3CHO+R2OH     3.4E11      0.     15.7E3 !
(397)<RAnZI94>!
C2H5OOH+R3OOH=>CH3CHO+R2OH+H2O2     8.0E11      0.     16.2E3 !
(398)<RAnZI94>!
C2H5OOH+R8CH3OO=>CH3CHO+R2OH+CH3OOH 1.1E12      0.     16.7E3 !
(399)<RAnZI94>!
C2H5OOH+R17C2H5OO=>CH3CHO+R2OH+C2H5OOH  1.1E12      0.     16.7E3 !
(400)<RAnZI94>!

!****** REACTIONS DE R18CH3COOO ****** !
R18CH3COOO+C2H4O#3=CH3COOOH+R13CH2CHO     1.0E12      0.      9.3E3 !
(401,-402)<RAnZI94>!
R18CH3COOO+R3OOH=CH3COOOH+O2              5.5E10      0.     -2.6E3 !
(402,-402)<COX90>!
R18CH3COOO+C2H5OOH=CH3COOOH+R17C2H5OO     5.0E11      0.      9.2E3 !
(403,-403)<RAnZI94>!
R18CH3COOO+C2H5OOH=>CH3CHO+R2OH+CH3COOOH  5.0E11      0.      9.2E3 !
(404)<RAnZI94>!
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R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2     1.7E12      0.     -1.0E3 !
(405)<CAVAnAGH90>!

!****** REACTIONS DE CH3COOOH ******!
CH3COOOH=>R4CH3+CO2+R2OH                  1.0E16      0.     40.0E3 !
(406)<CAVAnAGH90>!

!*******************************************************

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!*                                          Primary mechanism of the
oxidation of Ethanol                                    *!
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!*************************************!
!*           REACTIOnS OF ETHANOL      *!
!*************************************!

!Unimolecular initiation

C2H5OH(+M)=R11C2H5+R2OH(+M)       2.95E+22    -2.16        96.6E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /3.80E+88   -19.70       114.5E+3/
                          TROE   /2.094   16539    1.114   161.36/

C2H5OH(+M)=C2H4Z+H2O(+M)          4.90E+9     1.36    65.8E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /2.404+8    -17.9    84.8E+3/
                          TROE   /2.126     13568   0.969  160.4/

C2H5OH(+M)=R4CH3+R6CH2OH(+M)     6.61E+23  -2.16    88.04E+3
!Tsang, J Chem Kinet 36,436-63,2004!
                         LOW     /1.99E+85  -18.9    104.8E+3/
                         TROE    /2.058     16911    1.071   135.3/

C2H5OH(+M)=R23C2H4OH+R1H(+M)     2.01E+17    -0.149     101.8E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                         LOW     /4.902E+94   -21.65     123.1E+3/
!Reaction (c5),T=500-1800K
                        !LOW     /2.716E+83   -21.47     38.44E+3/
!Reaction (c5),T=1800-3000K
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C2H5OH(+M)=R24C2H4OH+R1H(+M)     7.54E+16    -0.275   94.05E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                          LOW     /7.708E+96   -22.47   116.9E+3/
!T=500-1800K
                         !LOW     /5.58E+82    -21.20   37824.5/
!T=1800-3000K
                          DUPLICATE

C2H5OH(+M)=R15C2H5O+R1H(+M)      2.70E+15    0.305    101.3E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!
                         LOW      /2.794E+88  -19.76    121.0E+3/
!T=500-1800K;
                        !LOW      /4.246E+91  -23.49    49435.8/
!T=1800-3000K,
                         DUPLICATE

!Bimolecular initiation

C2H5OH+O2=R23C2H4OH+R3OOH           2.100E+13      0.0     52400.0
C2H5OH+O2=R24C2H4OH+R3OOH           1.400E+13      0.0     46300.0
C2H5OH+O2=R15C2H5O+R3OOH            7.000E+12      0.0     55730.0

!Metatheses with abstraction of H-atom

!C2H5OH+R2OH=R23C2H4OH+H2O              6.203E+03      2.68      -576.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R23C2H4OH+H2O               3.60E+06       2.0        950.0
!Nancy, correlation Bozzelli 1999!

!C2H5OH+R2OH=R24C2H4OH+H2O              1.307E+05      2.43     -1456.6
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R24C2H4OH+H2O               2.40E+06       2.00     -2100.0
!Nancy, correlation Bozzelli 1999!

C2H5OH+R2OH=R15C2H5O+H2O                2.812E+02      2.97     -580.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H5OH+B1O=R23C2H4OH+R2OH               9.69E+02       3.23     4658.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007

C2H5OH+B1O=R24C2H4OH+R2OH               1.45E+05       2.47     876.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H5OH+B1O=R15C2H5O+R2OH                1.46E-03       4.73     1727.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H5OH+R1H=R23C2H4OH+H2                 1.88E+03       3.20     7150.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R24C2H4OH+H2                 1.79E+05       2.53     3420.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R15C2H5O+H2                  5.33E-23       10.58    -4459.0
!T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).
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!C2H5OH+R1H=R15C2H5O+H2                  5.36E+4        2.53     8753.6
!T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

!C2H5OH+R4CH3=R23C2H4OH+CH4              6.99E-83      30.14   -15663.0
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R23C2H4OH+CH4               3.30E+02       3.30    12291.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).

!C2H5OH+R4CH3=R24C2H4OH+CH4              1.02E-47      18.51    -9409.4
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R24C2H4OH+CH4               1.99E+01      3.37     7635.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

!C2H5OH+R4CH3=R15C2H5O+CH4               1.01E-51      19.68    -10323.5
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R15C2H5O+CH4                2.035E+0      3.57     7722.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

C2H5OH+R3OOH=R23C2H4OH+H2O2              4.2E+04        2.69     19080
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R24C2H4OH+H2O2              2.80E+04       2.69     15420
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R15C2H5O+H2O2            5.400E+04      2.0     15025.0    !
Grana et al.2010

C2H5OH+R11C2H5=R23C2H4OH+C2H6         1.500E+12      0.0     11700.0    !
Konnov 2005!

C2H5OH+R11C2H5=R24C2H4OH+C2H6         4.000E+13      0.0     10000.0    !
Konnov 2005!

C2H5OH+R11C2H5=R15C2H5O+C2H6          2.300E+04      2.0     10525.0    !
Grana et al.2010!

C2H5OH+R6CH2OH=R24C2H4OH+CH3OH        4.000E+11      0.0      9700.0    !
Konnov 2005!

C2H5OH+R7CH3O=R24C2H4OH+CH3OH         2.000E+11      0.0      7000.0    !
Konnov 2005!

C2H5OH+R15C2H5O=C2H5OH+R24C2H4OH      2.000E+11      0.0      7000.0    !
Konnov 2005!


!*************************************!
!*           REACTIOnS OF R23C2H4OH    *!
!*************************************!

R23C2H4OH=C2H4Z+R2OH                      3.52E-34      11.84   -18737.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                         1.35E+43      -10.29    28035.5
!at 1 atm, T=300-1000K
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!                                        7.93E+2        1.51     15180.3
!at 1 Torr, T=300-3000K
!                                        1.51E+33      -6.54     26960.4
!at 100 atm, T=300-1000K
!                                        4.90E-24       9.44    -12183.6
!at 100 atm, T=1000-3000K

R23C2H4OH=R1H+C2H3OH                     3.33E+28      -5.26     35586.9
!at 1 atm,T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                        2.67E+15      -1.92     29386.8
!at 1 Torr,T=300-3000K.
!                                        2.67E+27      -4.44     37208.5
!at 100 atm,T=300-3000K

R23C2H4OH=R24C2H4OH                   1.000E+11      0.0     39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81


R23C2H4OH+O2=C2H3OH+R3OOH        1.600E+12      0.0     5000.0

!*************************************!
!*           REACTIOnS OF R24C2H4OH    *!
!*************************************!

R24C2H4OH=CH3CHO+R1H                     8.34E+27       -5.19     35576.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                       8.96E+13       -1.61     28844.3
!at 1 Torr,T=300-3000K
!!                                       5.47E+27       -4.67     37685.4
!at 100 atm,T=300-3000K

R24C2H4OH=R1H+C2H3OH                     2.00E+28      -5.08     39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                       4.44E+21      -3.23     36570.6
!at 1 Torr,T=300-3000K
!!                                       1.22E+30      -5.17     41916.2
!at 100 atm,T=300-3000K

R24C2H4OH=R4CH3+HCHO                     1.14E+22       -3.59    34662.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                       5.92E+11       -1.04    28739.0
!at 1 Torr,T=300-3000K
!!                                       4.36E+23       -3.55    38679.0
!at 100 atm,T=300-3000K

R24C2H4OH+O2=CH3CHO+R3OOH                5.26E+17       -1.637    838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=CH3CHO+R3OOH               5.28E+17       -1.637    839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.

R24C2H4OH+O2=C2H3OH+R3OOH                5.33E+2        2.490     -402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=C2H3OH+R3OOH               7.62E+2        2.446     -296
!at 1 atm, T=300-2000K,Ref: DaSilva et al 2009, JphyschemA, 113,31.
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R24C2H4OH+R1H=CH3CHO+H2                  1.361E+09     1.29        2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=R6CH2OH+R4CH3              8.67E+16      -0.891      2903.3
!Rйaction (b2), Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=C2H3OH+H2                  4.896E+08      1.70       588.2
!Rйaction (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-
22.

R24C2H4OH+R1H(+M)=C2H5OH(+M)             3.607E+13       0.06      437.2
!Rйaction (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,
                                    LOW /2.767E+56     -15.72
10.7E+03/
                                   Duplicate

R24C2H4OH+R2OH=CH3CHO+H2O             1.500E+13      0.0         0.0
!Konnov 2005

R24C2H4OH+B1O=CH3CHO+R2OH                 9.040E+13      0.0         0.0
!Konnov 2005

!****************************************!
!*           REACTIOnS OF R15C2H5O     *!
!****************************************!

R15C2H5O=R4CH3+HCHO                       4.4E-29      10.69    -16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                       1.03E+23    -3.82     19303.7
!at 1 atm, T=300-1000K,
!!                                       2.71E+24    -4.50     21018.7
!at 1 Torr, T=300-1000K,
!!                                       1.87E-28    10.39    -12910.9
!at 1 Torr, T=1000-3000K,
!!                                       5.31E+21    -2.97     19560.1
!at 100 atm, T=300-1000K,
!!                                       9.56E-17    7.66      -7408.3
!at 100 atm, T=1000-3000K,

R15C2H5O=R1H+CH3CHO                       4.25E-32     11.49    -16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                       1.33E+38     -8.61    25513.8
!at 1 atm,T=300-1000K
!!                                       7.25E+31     -7.58    21370.4
!at 1 Torr,T=300-1000K
!!                                       2.14E-34     11.63    -15651.2
!at 1 Torr,T=1000-3000K
!!                                       2.61E+19     -2.15    21996.4
!at 100 atm,T=300-1000K
!!                                       1.64E-27     10.5     -15315.4
!at 100 atm,T=1000-3000K
```

```
R15C2H5O+O2=CH3CHO+R3OOH                6.0E+10       0.0        1.7E+3
!(287,-287)<BAULCH94>!

R15C2H5O+R2OH=CH3CHO+H2O                1.0E+13       0.0        0.0
!Marinov 1998

R15C2H5O+R1H=CH3CHO+H2                  7.47E+09      1.15       673.7
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22

R15C2H5O+R1H(+M)=C2H5OH(+M)             3.08E+11      0.894      12.9
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22
                                  LOW / 3.772E+51    -15.55
11.1E+3/
                                  DUPLICATE

R15C2H5O+B1O=CH3CHO+R2OH                1.210E+14     0.0        0.0
!Konnov 2005


!
*****************************************************************************
*****************************************************!
!
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*****************************************************!
!*                                          Secondary mechanism of the
oxidation of Ethanol                                  *!
!
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!
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!*************************************!
!*           REACTIONS OF C2H3OH       *!
!*************************************!

!C2H3OH+B1O=R13CH2CHO+R2OH               4.4E+10       0.7        3250.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+B1O=R13CH2CHO+R2OH                1.4E+13       0.0        2.3E3
!Acйtaldйhyde! (219,-219)<CAVAnAGH90>

!C2H3OH+R1H=R13CH2CHO+H2              2.700E+04     2.5
-1900.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R1H=R13CH2CHO+H2              1477.2        3.077
7230       !T=300-3000!RAO 2011! J Phys Chem 2011,115
!                                  REV   /1.41         3.721     24600/
C2H3OH+R1H=R13CH2CHO+H2                  1.31E+5       2.58       1220.0
!Acйtaldйhyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem
A,114,755-764.
```

```
!C2H3OH+R2OH=R13CH2CHO+H2O            1.500E+06     2.0
-1520.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R2OH=R13CH2CHO+H2O               2.300E+10     0.73     -1100.0
!Acйtaldйhyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2          3.200E+03     2.6
12400.0    !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R3OOH=R13CH2CHO+H2O2          1.626E+12     0.0
16295.1    !Syn_CH2H3OH! ajoutй le 20/10/2011 !Altarawneh et al 2011!
T=700-1300K!
C2H3OH+R3OOH=R13CH2CHO+H2O2             1.0E12        0.0       10.0E3
!Acйtaldйhyde!(311,-311)<CAVAnAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4           5.000E+10     0.0
7300.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R4CH3=R13CH2CHO+CH4              2.0E-6        5.6       2.5E+3
!Acйtaldйhyde! (216,-216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6             0.740         3.5       4140.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+R11C2H5=R13CH2CHO+C2H6           1.3E12        0.0       8.5E3
!Acйtaldйhyde! (218,-218)<HOHLEIn70>

C2H3OH=CH3CHO                           4.5E+06       1.8       5.1E+4
!Prof. Fournet
!!C2H3OH=CH3CHO                         8.590E+11     0.318     55900.00
! DaSilva 2006!
  !!                            REV/   1.050E+09     1.202
66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH              1.49E+05      1.67      6810.0
!P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29
C2H3OH+R1H=CH3CHO+R1H                   1.00E+13      0.00      1506.0
!T=300-2000K!form observation in Huynh et al 2009, j phys chem A
113,3177-3185:

!"The rate of this reaction is close to that of the H addition to C2H4:
C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+CO2+H2                1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5
!C2H3OH+R2OH=HCHO+R6CH2OH               1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5

!C2H4+OH<=>C2H3OH+H                     1.070E+04    2.600     4133.00
!Senosiain et al 2006
C2H4Z+R2OH=C2H3OH+R1H                   4.000E+12    0.000     4880.00
!Hippler et al 2000

!*************************************!
!*           REACTIOnS OF CH3CHO       *!
```

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!*************************************!

CH3CHO+R2OH=R14CH3CO+H2O                 2.300E+10   0.73
-1100.0     ! Konnov 2005!
CH3CHO+R1H=H2+R14CH3CO                   1.31E+5     2.58
1220.0      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
CH3CHO+R4CH3=R14CH3CO+CH4                2.0E-6      5.6
2.5E+3      !(216,-216)<BAULCH94>! T=300-1250K
CH3CHO+B1O=R14CH3CO+R2OH                 1.4E+13     0.
2.3E3       !(219,-219)<CAVAnAGH90>!
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO           8.1E10      0.
3.7E3       !(217,-217)<SCHERZER87>T=480-520K!NIST
CH3CHO+R11C2H5=C2H6+R14CH3CO             1.3E12      0.
8.5E3       !(218,-218)<HOHLEIn70>!
CH3CHO+R7CH3O=R14CH3CO+CH3OH             5.000E+12   0.0
0.0         !Konnov 2005!
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO         3.000E+12   0.0
11200.0     !Konnov 2005!

!CH3CHO+R2OH=R13CH2CHO+H2O               1.600E+13   0.0
2000.0      !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J
Chem Kin 2008,40,73-102
CH3CHO+R2OH=R13CH2CHO+H2O                3.370e+11   0.0
-619.98     !Mech Sandiego=ref:Juan Li's PhD thesis!
!CH3CHO+R1H=R13CH2CHO+H2                 4.40E+14    0.0
10.0E+3     !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R1H=R13CH2CHO+H2                  2.72E+03    3.1
5206.5      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
!CH3CHO+R4CH3=R13CH2CHO+CH4              6.00E+12    0.0
11000.0     !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R4CH3=R13CH2CHO+CH4               2.45E+1     3.15
5727.0      !Marinov 1998
CH3CHO+B1O=R13CH2CHO+R2OH                3.720E+13   -0.2
3556.0      !Marinov 1998




!****** REACTIONS DE C2H5 ******!
R11C2H5+R10C2H3V=>C4H8Y                    1.5E13      0.         0. !
(61,-61)<TSAnG86>!
!R11C2H5+R11C2H5=>C4H10                     1.1E13      0.         0. !
(65,-65)<BAULCH94>!


!****** REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE ******!

C2H3CHO+R2OH=CH2CHCO+H2O                   1.0E13      0.0    0.0    !
<MARInOV>!
C2H3CHO+B1O=CH2CHCO+R2OH                   7.2E12      0.0    2.0E3  !
<MARInOV>!
```

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C2H3CHO+B1O=CH2COZ+R5CHO+R1H              5.0E7       1.76   0.08E3 !
<MARInOV>!
C2H3CHO+R1H=CH2CHCO+H2                    4.0E13      0.0    4.2E3  !
<MARInOV>!
C2H3CHO+R1H=C2H4Z+R5CHO                   2.0E13      0.0    3.5E3  !
<MARInOV>!
C2H3CHO+O2=CH2CHCO+R3OOH                  3.0E13      0.0   38.5E3  !
<MARInOV99>+ MF correlation Baptiste
CH2CHCO=R10C2H3V+B2CO                     1.0E14      0.0   34.0E3  !
<MARInOV>!
CH2CHCO+B1O=R10C2H3V+CO2                  1.0E14      0.0    0.0    !
<MARInOV>!
C3H5Y+R3OOH=>C2H3CHO+R1H+R2OH              7.0E18     -2.0    0.0    !
<TSAnG91>!
C3H5Y+O2=C2H3CHO+R2OH                     1.8E13     -0.41   22.9E3 !
<BOZELLI93>!
C3H5Y+B1O=C2H3CHO+R1H                     1.8E14      0.0     0.0   !
<SLAGLE92>!

!*****************************************************!
!       REACTIONS DES ESPECES NON OXYGEnNS EN C3      !
!*****************************************************!

!****** REACTIONS DE C3H2  ***** (CHCCH(..))*****!

B4CH+C2H2=C3H2+R1H                        2.1E14       0.0        -0.5E3 !
<MILLER92/BAULCH94>!
C3H2+B1O=R9C2H+R1H+B2CO                   3.0E13       0.0         0.0   !
<PEETERS97>!
C3H2+R2OH=C2H2+R5CHO                      5.0E13       0.0         0.0   !
<MILLER92>!
C3H2+O2=R12CHCOZ+B2CO+R1H                 5.0E13       0.0         0.0   !
<MILLER92>!


!****** REACTIONS DE C3H3 ***** (CHCCH2(.)) Propargyl*****stablilise par
resonnance !

B6CH2+C2H2=C3H3+R1H                      1.8E14       0.0         0.0   !
<MILLER87/BAULCH94>!
C3H3+R1H=C3H2+H2                         2.0E13       0.0         0.0   !
<MILLER92/BRAUn89>!
C3H3+B1O=R9C2H+HCHO                      1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
C3H3+R2OH=C3H2+H2O                       2.0E13       0.0         0.0   !
<MILLER92>!
C3H3+R2OH=R10C2H3V+R5CHO                 4.0E13       0.0         0.0   !
<WAnG97>!
C2H2+R12CHCOZ=C3H3+B2CO                  1.0E11       0.0         3.0E3 !
<MILLER92>!
C3H3+O2=CH2COZ+R5CHO                     3.0E10       0.0         2.9E3 !
<MILLER92/SLAGUE88>!
C3H2+R1H=C3H3                            1.0E14       0.0         0.0   !
<est>!
```

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C3H3+R3OOH=>R2OH+R9C2H+HCHO              1.0E15      -0.8         0.0   !
<Heyberger>!
C3H3+C3H3=C6H6#                         1.0E12       0.0          0.0   !
<STEIn90>shocktube!
C3H3+C3H3=C6H5#+R1H                      1.0E12       0.0          0.0   !
<STEIn90>flame!



!****** REACTIONS DE pC3H4 ***** (CH3CCH) Propyne *****!

!pC3H4=>aC3H4                            2.1E12       0.0         60.0E3
     !<HIDAKA89>!
pC3H4+M=C3H3+R1H+M                       4.7E18       0.0         80.0E3
     !<HIDAKA89>!
C2H2+B5CH2=pC3H4                         3.5E12       0.0          0.0
     !<TSAnG86>!

pC3H4=R9C2H+R4CH3                        4.2E15      0.0        125.0E3  !
<KInGAS1500>!
pC3H4+O2=C3H3+R3OOH                      2.1E12      0.0         40.8E3  !
<est Ingham>!
pC3H4+R1H=C2H2+R4CH3                     1.3E5       2.5         1.00E3  !
<hidaka89> !
pC3H4+R1H(+M)=tC3H5(+M)                  8.5E12      0.0          1.7E3  !
<WAGnER72>!
                    LOW   /5.6E25     -7.27     6.58E3/
          !<Marinov97!
pC3H4+R1H(+M)=sC3H5(+M)                  5.8E12      0.0          3.1E3  !
     <WAGnER72>!
                    LOW   /3.8E25     -7.27     7.98E3/
          !<estimated>!
pC3H4+R4CH3=C3H3+CH4                     2.2E0       3.5          5.7E3  !
<asTSAnG91>!
pC3H4+R1H=C3H3+H2                        1.7E5       2.5          2.5E3  !
<asTSAnG91>

pC3H4+R9C2H=C3H3+C2H2                    3.6E12      0.0            0.0
     !<asTSAnG91>!
pC3H4+R10C2H3V=C3H3+C2H4Z                2.2E0       3.5          4.7E3  !
<asTSAnG91>!
pC3H4+R11C2H5=C3H3+C2H6                  2.2E0       3.5          6.6E3  !
<asTSAnG91>!
pC3H4+B1O=R12CHCOZ+R4CH3                 1.5E13      0.0          2.1E3  !
<WARnATZ84>!
pC3H4+B1O=R2OH+C3H3                      3.4E4       2.16         4.8E3  !
<<ADUSEI, G.Y, 1996>!
pC3H4+R2OH=CH2COZ+R4CH3                  4.3E11      0.0         -0.8E3  !
<BOODAGHIAnS87>!
pC3H4+R2OH=R1H+C2H3CHO                   4.3E11      0.0         -0.8E3  !
<asBOODAGHIAnS87>!
pC3H4+R2OH=C3H3+H2O                      3.1E6       2.0         -0.3E3  !
<asTSAnG91>!
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pC3H4+R3OOH=C2H4Z+B2CO+R2OH             6.0E9       0.0          8.0E3  !
as296<TSAnG86>!
pC3H4+R3OOH=C3H3+H2O2                   9.6E3       2.6         13.9E3  !
<asTSAnG91>!
pC3H4+R7CH3O=CH3OH+C3H3                 2.0E12      0.0          4.0E3  !
<Heyberger>!


!******** REACTIONS DE aC3H4 ***** (CH2CCH2) Allene  *******!

aC3H4=pC3H4                             2.5E12      0.0         59.0E3  !
<HIDAKA89>!
aC3H4+M=C3H3+R1H+M                      2.0E18      0.0         80.0E3  !
<HIDAKA89>!
aC3H4+O2=C3H3+R3OOH                     2.8E13      0.0         39.0E3  !
<Estimation Ingham>!
aC3H4+R1H(+M)=C3H5Y(+M)                       4.0E12      0.0
2.7E3      !<WAGnER72>!
                    LOW   /5.6E33       -5.0   4.44E3/
           !<Marinov97> !
aC3H4+R1H(+M)=tC3H5(+M)                 8.5E12      0.0          2.0E3  !
<WAGnER72>!
                    LOW   /1.1E34     -5.0     4.44E3/
           !<Marinov97!
C2H4Z+B4CH=aC3H4+R1H                    1.3E14      0.0         -0.3E3  !
<BAULCH94base>!
R10C2H3V+B5CH2=aC3H4+R1H                3.0E13      0.0          0.0    !
<MILLER92>!
iC4H3+B5CH2=aC3H4+R9C2H                 2.0E13      0.0          0.0    !
<MILLER92>!
aC3H4+B1O=R1H+B2CO+R10C2H3V             6.6E12      0.0          3.0E3  !
<Aleksandrev nist>!
aC3H4+R2OH=CH2COZ+R4CH3                 2.0E12      0.0         -0.2E3  !
<LIU88>!
aC3H4+R2OH=HCHO+R10C2H3V                2.0E12      0.0         -0.2E3  !
<LIU88>!

aC3H4+R1H=C3H3+H2                       1.3E6       2.53         9.2E3  !
<est.butatiene>!
aC3H4+B1O=C3H3+R2OH                     6.2E12      0.0          1.9E3  !
<fromAleksandrev nist>!
!d'aprиs leur vitesse de rйaction total et d'addition !
aC3H4+R2OH=C3H3+H2O                     6.2E6       2.0          0.4E3  !
<est.butadiene>!
aC3H4+R4CH3=C3H3+CH4                    2.0E12      0.0          7.7E3  !
<WU87>!
aC3H4+R9C2H=C3H3+C2H2                   1.0E13      0.0          0.0    !
<WU87>!
aC3H4+C3H5Y=C3H3+C3H6Y                  2.0E12      0.0          7.7E3  !
<DAGAUT92>
aC3H4+R7CH3O=CH3OH+C3H3                       4.0E12      0.0
9.6E3      !<correlations a partir de Heyberger>!
aC3H4+R11C2H5=C2H6+C3H3                    5.0E14      0.0        19.8E3
      !<asbutadiene>!
```

```
aC3H4+R10C2H3V=C2H4Z+C3H3              5.0E14      0.0        19.8E3   !
<asbutadiene>!
!aC3H4+R4CH3=C4H7T                      5.7E10      0.0         6.8E3  !
<Scherzer>!
!aC3H4+R4CH3=C4H7T                      3.4E11      0.0         7.4E3
     !<Tsang91x2>!
!aC3H4+R4CH3=iC4H7                      1.6E11      0.0         5.0E3
     !<Tsang73>!
!aC3H4+R4CH3=C4H7T                           0.8E11      0.0
7.4E3      !<Tsang91x2/4>!
aC3H4+R4CH3=iC4H7                       0.4E11      0.0         5.0E3
     !<Tsang73/3>!


!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K
(Tsang91)!
!aC3H4+C3H3=C6H6#+R1H                  1.4E12       0.0        10.0E3  !
<HIDAKA89>!


!******** REACTIONS DE cC3H4 ***** cyclopropene *********!

cC3H4=aC3H4                             1.5E14      0.0    50.5E3  !
<Karni>
cC3H4=pC3H4                             7.1E13      0.0    47.8E3  !
<Karni>
cC3H4+R1H=cC3H3+H2                      5.4E4       2.5    -1.9E3  !
<Heyberger>!
cC3H4+R2OH=cC3H3+H2O                    3.0E6       2.0    -1.5E3  !
<Heyberger>!
cC3H4+R2OH=C2H4Z+R5CHO                  2.8E12      0.0    -1.0E3  !
<Heyberger>!
cC3H3+R3OOH=R2OH+C2H2+R5CHO             1.0E15     -0.8     0.0    !
<Heyberger>!
cC3H3+R4CH3=cC4H6                       1.0E13      0.0     0.0    !
<estimation>!
cC3H3+R1H=cC3H4                         1.0E14      0.0     0.0    !
<estimation>!

!****** REACTIONS DE C3H5Y ***** (CH2CHCH2(.)) Allyl *****stablilise par
resonnance !

!C3H5Y+R1H=C3H6Y                        2.0E13      0.0         0.0  !
<TSAnG91>!
C3H5Y+R1H=aC3H4+H2                      1.8E13      0.0         0.0  !
TSANG 91!*
C3H5Y+R1H=C3H6Y                         1.0E14      0.0         0.0  !
<allara>!!


!rйaction importante pour la formation de propиne!
C3H5Y+R4CH3=aC3H4+CH4                   3.0E12     -0.32     -0.1E3    !
<TSAnG91>!
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C3H5Y+R4CH3=C4H8Y                       1.0E14     -0.32     -0.1E3    !
<TSAnG91>!
C3H5Y+R2OH=aC3H4+H2O                    6.03E12     0.0         0.0  !
Tsang 91!
!peu d'effet de fall off!
C3H5Y+R10C2H3V=aC3H4+C2H4Z              2.4E12      0.0         0.0  !
<TSAnG91>!
!C3H5Y+R11C2H5=aC3H4+C2H6               9.6E11      0.0       -0.1E3    !
<TSAnG91>!
C3H5Y+R11C2H5=aC3H4+C2H6                2.0E13      0.0       -0.1E3    !
<TSAnG91>MODIF!!!!!
C3H5Y+B1O=R10C2H3V+HCHO                 1.8E14      0.0         0.0  !
<SLAGLE90,LEUnG95>!
!processus non elementaire impliquant la formation-decomposition de
l'hydroperoxyde
!C3H5Y+C3H3=C6H6#+2R1H                  5.6E20     -2.535     1.7E3    !
<MARInOV97>!
C3H5Y+C3H5Y=aC3H4+C3H6Y                 8.4E10      0.0       -0.3E3    !
<TSAnG91>!


!****** REACTIONS DE sC3H5 ***** (CH3CHCH(.)) 2-methyl vinyl *****!

sC3H5=C3H5Y                            5.0E13      0.0        37.0E3 !
<WEISSMAn89>!
R4CH3+C2H2=sC3H5                       6.0E11      0.0       7.7E3 !
<BAULCH94>!

!****** REACTIONS DE tC3H5 ***** (CH3C(.)CH2) 1-methyl vinyl *****!

tC3H5+R1H=aC3H4+H2                      3.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5+R4CH3=aC3H4+CH4                   1.0E11      0.0         0.0   !
<DAGAUT90>!
tC3H5+R10C2H3V=aC3H4+C2H4Z              1.0E12      0.0         0.0   !
<LEUnG95>!
tC3H5+R11C2H5=aC3H4+C2H6                1.0E12      0.0         0.0   !
<LEUnG95>!
tC3H5+B1O=CH2COZ+R4CH3                  1.8E14      0.0         0.0   !
<LEUnG95>!
tC3H5+O2=R4CH3+B2CO+HCHO                4.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5=C3H5Y                             2.0E13      0.0        47.0E3 !
<Weissman89>!


!****** REACTIONS DE C3H6Y ***** (CH3CHCH2) propene *****!

C2H4Z+B6CH2=C3H6Y                       9.6E13      0.0         0.0  !
<BAULCH94>!
C2H4Z+B5CH2=C3H6Y                       3.2E12      0.0       5.1E3  !
<BAULCH94>!
!duplicate R10C2H3V+R4CH3=C3H6Y         2.5E13      0.0         0.0  !
<TSAnG86>!
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C2H4Z+R4CH3=C3H6Y+R1H                    6.6E11      0.0     15.9E3  !
<TSAnG86>!
R11C2H5+B6CH2=C3H6Y+R1H                  9.0E12      0.0       0.0   !
<TSAnG86>!
C2H6+B4CH=C3H6Y+R1H                      1.1E14      0.0     -0.3E3  !
<BAULCH94>!
C3H6Y+R1H=sC3H5+H2                       7.83E5      2.5    12.28E3  !
<TSAnG92>!
C3H6Y+R1H=tC3H5+H2                       3.9E5       2.5     5.82E3  !
<TSAnG92>!
C3H6Y+R1H=C3H5Y+H2                       1.7E5       2.5      2.5E3  !
<TSAnG91>!
C3H6Y+R4CH3=C3H5Y+CH4                    2.2E0       3.5      5.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=sC3H5+CH4                    8.4E-1      3.5     11.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=tC3H5+CH4                    1.3E0       3.5     12.9E3  !
<TSAnG91>!
C3H6Y+R11C2H5=C3H5Y+C2H6                 2.2E0       3.5      6.6E3  !
<TSAnG91>!
!C3H6Y+B1O=>CH2COZ+R1H+R4CH3             1.2E+5      2.56    -1130.0  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+B1O=C3H5Y+R2OH                     1.7E11      0.7      5.9E3  !
<TSAnG91>!
!C3H6Y+R2OH=HCHO+R11C2H5                 1.45E12     0.0      -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
!C3H6Y+R2OH=R4CH3+CH3CHO                 1.45E12     0.0      -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+R2OH=C3H5Y+H2O                     3.1E6       2.0      -0.3E3  !
<TSAnG91>!
C3H6Y+R2OH=sC3H5+H2O                     1.1E6       2.0     1.45E3  !
<TSAnG91>!
C3H6Y+R2OH=tC3H5+H2O                     2.1E6       2.0      2.8E3  !
<TSAnG91>!
C3H6Y+O2=C3H5Y+R3OOH                     1.9E12      0.0     39.0E3  !
<WALKER93>!
C3H6Y+R3OOH=C3H5Y+H2O2                   9.6E3       2.6     13.9E3  !
<TSAnG91>!

C3H6Y+R9C2H=pC3H4+R10C2H3V              1.2E13       0.0     0.0     !TSANG
91 mehdi!

!****** REACTIONS DE cC3H6 ***** cyclopropane *****!

cC3H6=C3H6Y                            4.6E14      0.0    62.6E3  !
<Hidaka87>!
cC3H6+R1H=C3H5Y+H2                      1.6E14      0.0   11.7E3   !
<Marshall86>!
cC3H6+R2OH=C3H5Y+H2O                         7.0E7       1.5    1.0E3   !
<Dobe82>!
cC3H6+R4CH3=C3H5Y+CH4                      2.0E11      0.0    9.6E3   !
<Exgas>!
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!****** REACTIONS DE R19C3H7 et iC3H7 ***** CH3CH2CH2(.) et  CH3CH(.)CH3
***** !

!R19C3H7 = R4CH3+C2H4Z                        6.400E+12   0.00    31000.0!!
ds мйса PRF
!R19C3H7 = R1H+C3H6Y                          3.000E+13   0.00   38000.00!!
ds мйса PRF
iC3H7 = R1H+C3H6Y                           6.000E+13   0.00   39000.00
R19C3H7 = iC3H7                               1.960E+10   1.00   38600.00
!R19C3H7+O2 =R3OOH+C3H6Y                       1.600E+12   0.00    5000.00
R19C3H7+O2 =R3OOH+C3H6Y                       3.7e16   -1.63    3420 !
2003DES/KLI4415-4427
iC3H7+O2 = R3OOH+C3H6Y                      1.400E+12   0.00    5000.00

!****** Propane (C3H8) chemistry ******!

R11C2H5+R4CH3=C3H8         3.4E13      0.          0.  !(59,-
59)<BAULCH94>!
C3H8+O2=>R3OOH+iC3H7         1.4E+0013  0.000  50323.7  ! BI 2 CN
C3H8+O2=>R3OOH+R19C3H7         4.2E+0013  0.000  53033.0  ! BI 3 CN
B1O+C3H8=>R2OH+iC3H7         2.6E+0013  0.000   5200.0  ! ME 15 CW
B1O+C3H8=>R2OH+R19C3H7         1.0E+0014  0.000   7850.0  ! ME 16 CW
C3H8+R1H=>H2+iC3H7           9.0E+0006  2.000   5000.0  ! ME 17 CW
!C3H8+R1H=>H2+R19C3H7           5.7E+0007  2.000   7700.0  ! ME 18 CW!!ds
мйса PRF
C3H8+R2OH=>H2O+iC3H7       2.6E+0006  2.000   -765.0  ! ME 19 CW
!C3H8+R2OH=>H2O+R19C3H7         5.4E+0006  2.000    450.0  ! ME 20 CW!!ds
мйса PRF
C3H8+R3OOH=>H2O2+iC3H7     4.0E+0011  0.000  15500.0  ! ME 21 CN
!C3H8+R3OOH=>H2O2+R19C3H7       1.2E+0012  0.000  17000.0  ! ME 22 CN!!ds
мйса PRF
C3H8+R4CH3=>CH4+iC3H7      2.0E+0011  0.000   9600.0  ! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7        6.0E-0001  4.000   8200.0  ! ME 24 CN!!ds
мйса PRF
C3H8+R5CHO=>HCHO+iC3H7     1.0E+0007  1.900  17000.0  ! ME 25 CN
C3H8+R5CHO=>HCHO+R19C3H7        2.0E+0005  2.500  18500.0  ! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7    2.0E+0011  0.000  11000.0  ! ME 33 CN
!C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! ME 34 CR!!ds
мйса PRF
C3H8+iC3H7=>C3H8+R19C3H7        8.4E-0003  4.200   8700.0  ! ME 35 CN
R1H+iC3H7=>C3H8             8.3E+0012  0.000      0.0  ! CO 36 K

!****************Reactions of Acetone*************************!
!R14CH3CO+R4CH3=>C2H6CO                    4.0E15     -0.8        0. !
(231,-231)<TSAnG86>!
R14CH3CO+R4CH3=>C2H6CO                     2.7E15     -0.8        0. !
(231,-231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low
pressure.
iC3H7+B1O=>C2H6CO+R1H                 1.0          0.0         0.0     !
Tsang88 (Nist)
C2H6CO+O2=>R3OOH+CH2COZ+R4CH3         4.2E12       0.0         49.28E3 !
Kingas!
C2H6CO+B1O=>CH2COZ+R4CH3+R2OH         1.02E14      0.0         7.85E3  !
Buda!
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C2H6CO+R1H=>CH2COZ+R4CH3+H2            5.70E07      2.0          7.70E3

C2H6CO+R2OH=>CH2COZ+R4CH3+H2O          5.34E06      2.0          0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4         6.00E-1      4.0          8.20E3

C2H6CO+R3OOH=>CH2COZ+R4CH3+H2O2        1.20E12      0.0          17.0E3

!*****************Reactions of Propanal***********************!

!R5CHO+R11C2H5=>C2H5CHO                    1.8E13       0.          0.
!(141,-141)<TSAnG86>!
!C2H5CHO=R5CHO+R11C2H5                     1.07E+14     0.0        62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240
R5CHO+R11C2H5=C2H5CHO                      3.4E+13      0.0        0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R5CHO+R11C2H5                     2.45E+15     0.0        72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)
R13CH2CHO+R4CH3=C2H5CHO                   3.4E+13      0.0        0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R4CH3+R13CH2CHO                   7.00E+15     0          81703
!Baulch et al 1992,J. Phys.Chem.Ref.Data 21 411–429.
B1O+C3H6Y=>C2H5CHO                         1.000E+12    0          5000.0
!Mech Franssoldati
!C2H5CHO+R1H=H2+B2CO+R11C2H5               4.0E13       0.0        4.2E3
!<Heyberger>! ADZ 714
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5             4.0E12       0.0        0.5E3
!<Heyberger>! ADZ 715

!C2H5CHO=R4CH3+R13CH2CHO                   2.00E+16     0          83800.
!Mech Franssoldati
C2H5CHO+R1H=H2+R25C2H5CO                   1.17E+11     0.0        6000
!Decottignies et al.2002.
C2H5CHO+B1O=R2OH+R25C2H5CO                 5.000e+12    0.0
1.790e+03  !Curran et al. Fuel (2011) 90(1) 331–338.
C2H5CHO+R2OH=H2O+R25C2H5CO                 2.690e+10    0.760
-3.400e+02  !Curran et al. Fuel (2011) 90(1) 331–338.
R25C2H5CO=B2CO+R11C2H5                     2.95E+12     0.0        11100.0
!Decottignies et al.2002.

!*************************************************

!*************************************************


!************************************************!
!     REACTIONS DES ESPECES NON OXYGENES EN C4     !
!************************************************!

!****** REACTIONS DE C4H2  ***** (CH///CC///CH) diacetylene ***** !

R9C2H+R9C2H=C4H2                       1.8E13       0.0         0.0   !
<TSAnG86>!
2C2H2=C4H2+H2                          1.5E13       0.0       42.7E3     !
<LEUnG95>!
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C2H2+R9C2H=C4H2+R1H                    9.0E13       0.0          0.0   !
BAULCH94!
!C4H2+R1H=C2H2+R9C2H                   6.0E14       0.0       15.4E3     !
<MEREDITH86>!
C4H2+R2OH=>R5CHO+C3H2                   6.7E12       0.0       -0.4E3    !
<LEEDS-website>!
C4H2+O2=R12CHCOZ+R12CHCOZ              9.6E12       0.0       31.1E3     !
<HIDAKA02>!!!
C4H2+R9C2H=>C6H2+R1H                   4.0E13       0.0          0.0   !
<MEREDITH86>!
C6H2+R1H=>C4H2+R9C2H                   9.3E14       0.0       15.1E3     !
<MEREDITH86>!

!****** REACTIONS DE nC4H3  ***** (ĽCH//CHC///CH) **********!

nC4H3(+M)=C4H2+R1H(+M)                 1.0E14       0.0       36.0E3     !
<MILLER92>!
          LOW   /1.0E14 0.0 30E3/
          TROE / 1.0  1.0  1.0E8/
C3H3+B4CH=nC4H3+R1H                    7.0E13       0.0          0.0   !
<MILLER92>!
!C3H3+B4CH=nC4H3+R1H                   5.0E13       0.0          0.0   !
<MILLER92>!
R9C2H+R10C2H3V=nC4H3+R1H               1.8E13       0.0          0.0   !
<TSAnG86>!
nC4H3+R1H=iC4H3+R1H                    2.4E11       0.79      2.41E3     !
<WAnG97>20Torr!
nC4H3+R1H=C4H2+H2                      0.6E13       0.0          0.0   !
<0.5*la cst de la react(c2h3+h)>!
2C2H2=nC4H3+R1H                        1.0E12       0.0       64.1E3   !
<LEUnG95>!
nC4H3+R2OH=C4H2+H2O                    1.5E13       0.0          0.0   !
<0.5* la cst de la react(c2h3+oh)>!
!***
!nC4H3+C2H2=C6H4#+R1H                   1.64E9       0.73      12.2E3   !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=C6H4#+R1H                  3.0E-11      6.48       6.6E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H4+R1H                   29.6         3.33       9.6E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H4+R1H                  2.77E-7      5.59       6.0E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H5                       1.73E11     -0.41       4.0E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H5                      6.17E15     -1.51       4.8E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=C6H5#                       3.33E24     -3.89       9.2E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=C6H5#                      7.0E14      -0.86       6.4E3      !
<WESTMORELAnD89, p=101kPa>!
!***
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!****** REACTIONS DE iC4H3  ***** (CH2//CĽC///CH) *****

iC4H3=nC4H3                             1.5E13       0.0      67.8E3   !
<LEUnG95>!
iC4H3(+M)=C4H2+R1H(+M)                  1.0E14       0.0      55.0E3     !
<MILLER92>!
           LOW  /2.0E15 0.0 48E3/
           TROE /1.0  1.0  1.0E8/
C3H2+B5CH2=iC4H3+R1H                    1.2E14       0.0       0.8E3     !
as(7)<BAULCH94>!
iC4H3+R1H=2C2H2                         2.40E19      -1.6       2800   !
<WAnG97>20Torr! !
C3H3+B4CH=iC4H3+R1H                     7.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R1H=C4H2+H2                       1.2E13       0.0         0.0   !
<equiv a la cst de la react(c2h3+h)>!
iC4H3+B1O=CH2COZ+R9C2H                  2.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R2OH=C4H2+H2O                     3.0E13       0.0         0.0   !<
equiv a la cst de la react(c2h3+oh)>!
iC4H3+O2=CH2COZ+R12CHCOZ                1.0E12       0.0         0.0   !
<MILLER92>!
*
iC4H3+R10C2H3V=2C3H3                    4.0E12       0.0         0.0   !
MILLER 92 !
iC4H3+R10C2H3V=>lC6H5+R1H                6.0E12       0.0         0.0   !
MILLER 92!

!****** REACTIONS DE C4H4  ***** (CH2//CHC///CH) vinylacetylene *****!

C3H3+B5CH2=C4H4+R1H                     4.0E13       0.0           0.0 !
<MILLER92>!
R10C2H3V+C2H2=>C4H4+R1H                 2.0E13       0.0        25.1E3 !
(40,-40)<DOUTE95>!
C4H4+R1H=>R10C2H3V+C2H2                 2.0E13       0.0        12.4E3 !
<DOUTE95>
C2H4Z+R9C2H=C4H4+R1H                    1.2E13       0.0           0.0 !
(50,-50)<TSAnG86>!
C4H4+R1H=nC4H3+H2                       2.0E7        2.0         15.E3 !
<Miller 92>!
C4H4+R1H=iC4H3+H2                       3.0E7        2.0          5.E3 !
<Miller 92>!
R9C2H+C4H4=>C2H2+iC4H3                  4.0E13       0.0           0.0 !
<MEREDITH86>!
C2H2+iC4H3=>R9C2H+C4H4                  3.0E13       0.0        27.9E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+nC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
nC4H3+C2H4Z=>R10C2H3V+C4H4              3.5E11       0.0        13.4E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+iC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
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iC4H3+C2H4Z=>R10C2H3V+C4H4           1.3E11       0.0        24.1E3 !
<MEREDITH86>!
C4H4+C2H2=C6H5#+R1H                  1.0E09       0.0       30.02E3 !
BENSON  !MF
C4H4+R10C2H3V=C6H6#+R1H              1.9E12       0.0         2.5E3 !
<LInSTEDT96>!
C4H4+B1O=aC3H4+B2CO                  3.0E13       0.0         1.8E3 !
<LEUnG95>!
C4H4+B1O=pC3H4+B2CO                  2.7E13       0.0         1.8E3 !
<MILLER>!
C4H4+R2OH=nC4H3+H2O                  7.5E6        2.0         5.0E3 !
<MILLER92>!
C4H4+R2OH=iC4H3+H2O                  1.0E7        2.0         2.0E3 !
<MILLER92>!
aC3H4+aC3H4=C2H4Z+C4H4               1.0E15       0.0        48.0E3 !
<HIDAKA89>!


!****** REACTIONS DE tC4H4  ***** (CH2//C//C//CH2) *****!

tC4H4+R2OH=iC4H3+H2O                 2.0E7        2.0         2.0E3   !
<Marinov>!
tC4H4+R1H=iC4H3+H2                   3.0E7        2.0         6.0E3   !
<Marinov>!

!****** REACTIONS DE nC4H5  ***** (ĽCH//CHCH//CH2) *****

nC4H5(+M)=R1H+C4H4(+M)               1.0E14       0.0       37.0E3      !
<MILLER92>!
            LOW   /1.00e+14 0.0 30000/
nC4H5+R1H=C4H4+H2                    1.5E13       0.0          0.0    !
<WAnG97>!
nC4H5+R1H=iC4H5+R1H                  1.0E14       0.0          0.0    !
<MILLER92>!
nC4H5+R4CH3=C5H8                     1.0E13       0.0          0.0    !
<estimated> !

nC4H5=C2H2+R10C2H3V                  1.0E14       0.0       43.9E3      !
<HIDAKA96>!
!***
!MF car lC6H6 n'intervient qu'ici
!nC4H5+C2H2=lC6H6+R1H                 1.17E-15     7.84        2.0E3  !
<WESTMORELAnD89, p=2.6kPa>!
!nC4H5+C2H2=lC6H6+R1H                 3.47E-15     7.73        2.5E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H6#+R1H                  1.90E7       1.47        4.2E3  !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H6#+R1H                 2.38E8       1.18        3.7E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=lC6H7                      8.74E12     -1.27        3.6E3 !
<WESTMORELAnD89, p=2.6kPa>!
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nC4H5+C2H2=lC6H7                    7.24E14     -1.38       4.0E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H7#                     1.96E19     -3.35       5.2E3 !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H7#                    7.12E21     -3.64       6.3E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H7+R1H             8.28E-28    11.89       5.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H7+R1H            3.55E-43    16.16      -0.2E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H8                 2.90E15     -0.78       1.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H8                1.50E13     -0.075      0.1E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H8#                 5.50E15     -1.67       1.5E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H8#                8.53E13     -1.11       0.8E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H6#+H2              2.80E-7      5.63      -1.9E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H6#+H2             1.84E-13     7.07      -3.6E3 !
<WESTMORELAnD89, p=101kPa>!
!***
nC4H5+R2OH=C4H4+H2O                  2.5E12       0.0          0.0  !
<WAnG97>!

!nC4H5+O2=R5CHO+C2H3CHO               1.7e29      -5.31       6.5E3 !MF
as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>
nC4H5+O2=R5CHO+C2H3CHO              5.67E28      -5.31       6.5E3 !MF
nC4H5+O2=C2H4Z+B2CO+R5CHO           1.13e29      -5.31       6.5E3 !MF
nC4H5+O2=C4H4+R3OOH                 5.19E15       -1.26        3.31e3  !
MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>

 !****** REACTIONS DE iC4H5  ***** (CH2//CHCH//CH2) *****stablilise par
resonnance
iC4H5=nC4H5                         1.5E13       0.0        67.8E3 !
<LEUnG95>!


iC4H5(+M)=R1H+C4H4(+M)              1.0E14       0.0        50.0E3 !
<MILLER92>!
            LOW   /2.0E15 0.0 42000/
iC4H5+R1H=C4H4+H2                   3.0E13       0.0          0.0  !
<WAnG97>!
iC4H5+R4CH3=iC5H8                   1.0E13       0.0          0.0  !
<estimated> !
2R10C2H3V=iC4H5+R1H                 1.5E30      -4.95       13.0E3  !
<WAnG97>20Torr!
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!***2R10C2H3V=iC4H5+R1H                1.2E22      -2.44       13.7E3  !
<WAnG97>760Torr!
iC4H5+R2OH=C4H4+H2O                    5.50E12      0.0          0.0  !
<WAnG97>!
iC4H5+O2=HCHO+CH2CHCO                  4.5E16      -1.39        1.0E3  !
estimй par{O2+C2H3=HCHO+CHO}!
iC4H5+O2=C4H4+R3OOH                    1.34E6       1.61         -400  !
estimй par {O2+C2H3=C2H2+OOH}!


!****** REACTIONS DE C4H5-1s  ***** (CH3/CHЃ/C///CH) *****stablilise par
resonnance

!C4H5-1s=R1H+C4H4                        3.0E13       0.0        45.0E3 !
<HIDAKA96>!
C4H5-1s=R1H+C4H4                         6.0E13       0.0        50.4E3 !
add inverse!
! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-1s+R1H=C4H4+H2                      2.0E13       0.0         0.0   !
<MILLER92/BRAUn89>!
C4H5-1s+B1O=R9C2H+CH3CHO                 1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
C4H5-1s+R2OH=C4H4+H2O                    2.0E13       0.0         0.0   !
<MILLER92>!
C4H5-1s+R2OH=R5CHO+sC3H5                 4.0E13       0.0         0.0   !
<WAnG97>!
C4H5-1s+O2=R5CHO+B2CO+C2H4Z              3.0E10       0.0         2.9E3 !
<MILLER92/SLAGUE88>!
C4H5-1s+C4H5-1s=C8H10#                   1.0E12       0.0         0.0   !
<STEIn90>shocktube!

!****** REACTIONS DE C4H5-1p  ***** (CH2Ѓ/CH2/C///CH) *****

!C4H5-1p=R1H+C4H4                         3.0E13       0.0        45.0E3 !
<HIDAKA96>!
!C4H5-1p=R1H+C4H4                         4.0E13       0.0        38.8E3 !
<HIDAKA96>!
C4H5-1p=R9C2H+C2H4Z                      2.0E14       0.0        57.0E3 !
<HIDAKA96>!
C4H5-1p+O2=C4H4+R3OOH                    1.6E12       0.0         5.0E3 !
PAG00!
C4H5-1p=C4H5-1s                          5.0E12       0.0        37.4E3 !
PAG00!

!****** REACTIONS DE C4H5-2  ***** (CH3/C///C/CH2Ѓ) *****stablilise par
resonnance

!C4H5-2=R1H+tC4H4                        3.0E13       0.0       50.0E3 !
<fromHIDAKA96+5!
C4H5-2=R1H+tC4H4                         6.0E13       0.0       54.3E3 !
toto!

!C4H5-2=iC4H5                            3.0E13       0.0       50.0E3 !
<fromHIDAKA96>!
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C4H5-2=iC4H5                              5.0E12       0.0       50.5E3 !
PAG00!
C4H5-2+C4H5-2=C8H10#                      1.0E12       0.0          0.0 !
<STEIn90>shocktube!

! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-2+B1O=C3H3+HCHO                    1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
C4H5-2+R2OH=R10C2H3V+B2CO+R4CH3         4.0E13       0.0         0.0   !
<WAnG97>!
C4H5-2+O2=CH2COZ+B2CO+R4CH3             3.0E10       0.0         2.9E3 !
<MILLER92/SLAGUE88>!


!****** REACTIONS DE C4H6Z2  ***** 1,3 Butadiene (CH2CHCHCH2) *****!
!R10C2H3V+R10C2H3V=C4H6Z2              6.8E12       0.0         0.0   !
<TSAnG86 P=2.6KPa T=1500>!
R10C2H3V+R10C2H3V=C4H6Z2              9.8E14      -0.5         0.0   !
<HIDAKA96shocktube>!
!
C4H6Z2=C4H4+H2                         2.5E15       0.0      94.7E3   !
<HIDAKA96>
C4H6Z2=iC4H5+R1H                      1.4E15       0.0      98.0E3   !
<HIDAKA96>!
!
C2H4Z+R10C2H3V=C4H6Z2+R1H             5.0E11       0.0       7.3E3   !
<TSAnG86>!
!
C4H6Z2+R1H=nC4H5+H2                    1.3E6        2.53     12.2E3   !
<WAnG97>!
C4H6Z2+R1H=iC4H5+H2                    6.6E5        2.53      9.2E3   !
<WAnG97>!
!
!C4H6Z2+R1H=C4H7-1               2.6E13       0         3.2E3   !
ESTIMATED *2!
!C4H6Z2+R1H=C4H7Y                2.6E13       0        1.56E3   !
ESTIMATED *2!
C4H6Z2+R1H=C4H7-1                  1.3E13       0         3.2E3   !
ESTIMATED
C4H6Z2+R1H=C4H7Y                   1.3E13       0        1.56E3   !
ESTIMATED !
!
C4H6Z2+R4CH3=nC4H5+CH4                 7.0E13       0.0      18.5E3   !
<WU87>!
C4H6Z2+R4CH3=iC4H5+CH4                 7.0E13       0.0      15.5E3   !
<WU87-3kcal>!
!C4H6Z2+R4CH3=C5H9Y              6.3E10       0.0      7.49E3   ! PERRIN
88 nist!
!C4H6Z2+R4CH3=iC5H9              1.8E11       0.0       8.0E3   !
Estimated*2!
C4H6Z2+R4CH3=C5H9Y                 6.31E10      0.0      7.49E3   !
PERRIN 88 nist!
C4H6Z2+R4CH3=iC5H9                 9.64E10      0.0       8.0E3   !
Estimated!
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```
!
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z          5.0E14       0.0      22.8E3   !
<HIDAKA96>!
C4H6Z2+R10C2H3V=iC4H5+C2H4Z          5.0E14       0.0      19.8E3   !
<HIDAKA96-3kcal>!
!
C4H6Z2+B1O=C3H5Y+R1H+B2CO            6.0E08       1.45      0.9E3   !
<LEUnG95,BREZInSKY84>!
!
R10C2H3V+C4H6Z2=C6H8#+R1H           7.4E014     -0.66     8.42E3   !
<frenklach >!
!R10C2H3V+C4H6Z2=C6H8#+R1H           2.28E12     -0.24      9.9E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H8#+R1H            4.15E-11     6.39      2.4E3   !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+C4H6Z2=lC6H8+R1H           1.0E10       1.05     14.0E3     !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H8+R1H            2.48E-15     8.20      6.3E3    !
<WESTMORELAnD89, p=101kPa>!
!***
C4H6Z2+C2H2=C6H8#                    2.3E12       0.0      35.0E3     !
<WESTMORELAnD89>!
!***
!MF car lC6H9 n'intervient qu'ici
!R10C2H3V+C4H6Z2=lC6H9                5.48E28     -5.31      9.3E3     !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H9                 1.48E12     -0.17      3.2E3    !
<WESTMORELAnD89, p=101kPa>!
!***
R10C2H3V+C4H6Z2=C6H9Z#              1.64E29     -6.12      9.6E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H9Z#                7.06E13     -1.35      4.0E3   !
<WESTMORELAnD89, p=101kPa>!
!***
C4H6Z2+C2H4Z=C6H10#                  2.3E10       0.0      27.0E3   !
<WESTMORELAnD89>!

C4H6Z2+R2OH=nC4H5+H2O                6.2E6        2.0       3.4E3     !
<WAnG97>!
C4H6Z2+R2OH=iC4H5+H2O                3.1E6        2.0       0.4E3     !
<WAnG97>!
C4H6Z2+R2OH=C3H5Y+HCHO               2.8E12       0.0      -0.9E3     !
<LInSTEDT96>!
C4H6Z2+R2OH=CH3CHO+R10C2H3V          5.6E12       0.0      -0.9E3     !
<fromLInSTEDT96>!
C4H6Z2+O2=iC4H5+R3OOH                4.0E13       0.0      57.9E3     !
<LEUnG95>!
C4H6Z2+C3H3=nC4H5+aC3H4              1.0E13       0.0      22.5E3     !
<HIDAKA96>!
C4H6Z2+C3H3=iC4H5+aC3H4              1.0E13       0.0      19.5E3     !
<HIDAKA96-3kcal>!

!****** REACTIONS DE C4H6-12  ***** (1,2) Butadiene (CH2CCHCH3) *****
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!C4H6-12=C4H6Z2                        3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-12=iC4H5+R1H                     4.2E15       0.0        92.6E3 !
<LEUnG95>!
!C4H6-12+R1H=R10C2H3V+C2H4Z            4.0E11       0.0           0.0 !
<LEUnG95>!
!C4H6-12=C3H3+R4CH3                    7.3E14       0.0        75.4E3 !
<kingas1500K>!
!C4H6-12+R1H=C4H7-2                    1.3E13       0.0         1.6E3 !
<heyberger> !
!C4H6-12+R1H=C4H7Y                     1.2E11       0.69        3.0E3 !
<heyberger>!
!C4H6-12+R1H=C4H7T                     1.3E13       0.0         3.2E3 !
<heyberger> !
!C4H6-12+R1H=iC4H5+H2                  1.7E5        2.5         2.5E3 !
<asTSAnG91>!
!C4H6-12+R4CH3=iC4H5+CH4               2.2E0        3.5         5.7E3 !
<asTSAnG91>!
!C4H6-12+R11C2H5=iC4H5+C2H6            2.2E0        3.5         6.6E3 !
<asTSAnG91>!
!C4H6-12+B1O=iC4H5+R2OH                1.7E11       0.7         5.9E3 !
<asTSAnG91>!
!C4H6-12+R2OH=iC4H5+H2O                3.1E6        2.0        -0.3E3 !
<asTSAnG91>!
!C4H6-12+R3OOH=iC4H5+H2O2              9.6E3        2.6        13.9E3 !
<asTSAnG91>!


!****** REACTIONS DE (c-C4H6)  ***** methyl-cyclopropene  *****

!B6CH2+pC3H4=cC4H6                      1.8E14       0.0         0.0   !
<LEUnG95>!
!cC4H6=C4H6Z2                          3.0E13       0.0        42.3E3 !
<LEUnG95>!
!cC4H6=C4H6-12                         3.0E13       0.0        43.8E3 !
<LEUnG95>!

!****** REACTIONS DE (C4H6-1) *****  1 Butyne *****

!C4H6-1=C4H6-12                        2.5E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-1=C4H5-1s+R1H                    7.7E14       0.0        87.9E3 !
Kinga&dH Melius!
!C4H6-1=C4H5-1p+R1H                    9.1E14       0.0        99.6E3 !
Kingas!
!C4H6-1=>C3H3+R4CH3                    3.0E15       0.0        75.8E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                1.3E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R11C2H5+C2H2               6.5E4        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                3.2E12       0.0         1.7E3 !
<asWAGnER72>!
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!C4H6-1+R1H=R11C2H5+C2H2              3.2E12       0.0         1.7E3 !
<asWAGnER72>!
! Les rйactions suivantes sont deduites de celles de 1-C4H8 generes par
EXGAS
!C4H6-1+R1H=H2+C4H5-1s                5.4E4        2.5        -1.9E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1s             1.5E12       0.0         7.1E3 !
<EXGAS>!
!C4H6-1+B1O=R2OH+C4H5-1s              8.8E10       0.7         3.2E3 !
<EXGAS>!
!C4H6-1+R2OH=H2O+C4H5-1s              3.0E6        2.0        -1.5E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1s            1.4E12       0.0        36.0E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s             1.4E12       0.0        41.4E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s            4.2E12       0.0        49.5E3 !
<DAGAUT90sec>!
!C4H6-1+R3OOH=>H2O2+C4H5-1s           6.4E3        2.6        12.4E3 !
<EXGAS>!
! Les rйactions suivantes sont deduites de celles generes par EXGAS pour
H primaires
!C4H6-1+R1H=H2+C4H5-1p                2.9E7        2.0         7.7E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1p             3.7          4.0         8.2E3 !
<EXGAS>!MF
!C4H6-1+B1O=R2OH+C4H5-1p              5.1E13       0.0         7.8E3 !
<EXGAS>!
!C4H6-1+R2OH=>H2O+C4H5-1p             2.7E6        2.0        -0.4E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1p             1.2E13       0.0        49.0E3 !
<EXGAS>!
!C4H6-1+R3OOH=>H2O2+C4H5-1p           6.0E11       0.0        17.0E3 !
<EXGAS>!
! Les rйactions d'addition suivantes sont deduites de celles de pC3H4
!C4H6-1+B1O=R12CHCOZ+R11C2H5          1.5E13       0.0         2.1E3 !
<asWARnATZ84>!
!C4H6-1+R2OH=CH2COZ+R11C2H5           4.3E11       0.0        -0.8E3 !
<asBOODAGHIAnS87>!

!***** REACTIONS DE (C4H6-2)***** 2 Butyne  *****

!C4H6-2=C4H6Z2                        3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-2=C4H6-12                       3.0E13       0.0        67.0E3 !
<HIDAKA96>!
!C4H6-2=C4H5-2+R1H                    2.0E14       0.0        87.3E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4              2.6E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4               6.5E12       0.0         1.7E3 !
<asWAGnER72>
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! Les rйactions suivantes sont deduites de celles de pC3H4
!C4H6-2+R1H=C4H5-2+H2                    3.4E5        2.5         2.5E3 !
<asTSAnG91*2>!
!C4H6-2+R4CH3=C4H5-2+CH4                 4.4E0        3.5         5.7E3 !
<asTSAnG91*2>!
!C4H6-2+B1O=B2CO+R10C2H3V+R4CH3          1.5E13       0.0         2.1E3 !
<asWARnATZ84>!
!C4H6-2+B1O=R2OH+C4H5-2                  1.2E11       0.7         7.6E3 !
<asTSAnG91*2>!
!C4H6-2+R2OH=B2CO+C2H4Z+R4CH3            4.3E11       0.0        -0.8E3 !
<asBOODAGHIAnS87>!
!C4H6-2+R2OH=C4H5-2+H2O                  6.2E6        2.0        -0.3E3 !
<asTSAnG91*2>!
!C4H6-2+O2=C4H5-2+R3OOH                  4.2E12       0.0        44.0E3 !
<InGHAM95*2>+4!
!C4H6-2+R3OOH=C4H5-2+H2O2                1.9E4        2.6        13.9E3 !
<asTSAnG91*2>!


!******* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y                            3.34E09       1.0      39.1E3  !
ESTIMATED !
!C4H7-1=C4H7V                            3.3E9         1.0      20.7E3  !
Estimated!
!C4H7-1=C2H4Z+R10C2H3V                   2.0E13        0.0      35.5E3  !
Estimated!
!C4H7-1+R4CH3=C5H10                      2.0E13        0.0         0.0  !
Estimated !
!C4H7-1+R1H=C4H8Y                        1.0E14        0.0         0.0  !
Estimated!

!******* Reactions de C4H7Y (CH3-CH.-CH=CH2)!*****stablilise par
resonnance
!C4H7Y+R1H=C4H8Y                         2.0E13        0.0         0.0  !
asTSANG 91!!
!C4H7Y+R1H=H2+C4H6Z2                     0.9E13        0.0         0.0  !
asTSANG 91!!
!C4H7Y+R1H=H2+C4H6-12                    0.9E13        0.0         0.0  !
asTSANG 91!
!C4H7Y+R3OOH=R2OH+C2H3CHO+R4CH3          1.0E15       -0.8         0.0  !
<Heyberger>!
!C4H7Y+R4CH3=iC5H10                      0.5E13        0.0         0.0  !
Estimated !

!**************Reactions de C4H7V (CH3-CH2-CH=CH.)*******!
!C4H7V=C4H7Y                            1.9E10         1.0      36.3E3  !
Heyberger!
!C4H7V=R11C2H5+C2H2                      2.0E13        0.0      33.0E3  !
Heyberger!

!**************Reactions de C4H7-2 (CH3-C.=CH-CH3)*****!
!C4H7-2=C4H7Y                          2.9E10     1.0        37.8E3  !
ESTIMATED !
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!C4H7-2=R4CH3+pC3H4                    2.0E13      0.0     31.5E3  !
ESTIMATED !

!**************Reactions de C4H7T (CH2=C.-CH2-CH3)********!

!C4H7T=C4H7-1                          3.34E09      1.0      40.6E3   !
ESTIMATED !
!C4H7T=C4H7Y                           2.0E13       0.0      47.0E3   !
<Heyberger>!
!C4H7T=R4CH3+aC3H4                     2.0E13       0.0      32.5E3   !
ESTIMATED !

!**************Reactions du 1-butene!

!C4H8Y+O2=C4H7Y+R3OOH                  3.6E12       0.0        38.2E3  !
<Heyberger>!
!C4H8Y+R1H=C4H7Y+H2                    5.4E4        2.5        -1.9E3  !
<Heyberger>!
!C4H8Y+R2OH=>HCHO+R4CH3+C2H4Z          1.4E12       0.0        -1.0E3  !
<Heyberger>!
!C4H8Y+R2OH=R4CH3+C2H5CHO              1.4E12       0.0        -1.0E3  !
<Heyberger>!!ds мйса PRF
!C4H8Y+R2OH=C4H7Y+H2O                  3.0E6        2.0       -1.52E3  !
<Heyberger>!
!C4H8Y+R4CH3=C4H7Y+CH4                 1.0E11       0.0         7.3E3  !
<Heyberger>!

!C2H5CHO+R1H=H2+B2CO+R11C2H5           4.0E13       0.0         4.2E3  !
<Heyberger>!
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5         4.0E12       0.0         0.5E3  !
<Heyberger>!

!***********reactions de iC4H8********!
!iC4H8+R2OH=iC3H7+HCHO                 1.4E12       0.0     -1040.0    !
(idem RF)
!iC4H8+R1H=>iC4H7+H2                   3.5E5        2.5        2510    !
(idem RF)
!iC4H8+R2OH=>iC4H7+H2O                 6.0D+06    2.000      -298.0    !
MES 878<C.M.>!(idem RF)
!iC4H7+R1H=iC4H8                       1.0E14       0.0         0.0    !
<estimation>!
!iC4H7+R3OOH=>R2OH+HCHO+tC3H5          1.0E15      -0.8          0.0    !
<Heyberger>!


!
**********************************************************************
**!
!
**********************************************************************
*********!
!*              MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE
*!
```

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!*
*!
!*    efficiency  coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
*********************************************************************
*********!
!*           PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
*********************************************************************
*********!


!REACTIONS OF BENZENE MOLECULES!
!***Umimolecular inititiation!
C6H5#+R1H(+M)=C6H6#(+M)             1.0E14      0.0        0.0      !
<WANG97>!
                          LOW   /6.6E75  -16.3   7.0E3/
                          TROE /1.0 0.1 585 6113/
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
!***Bimolecular inititiation!
C6H6#+O2=C6H5#+R3OOH               6.0E13      0.0          63.4E3   !
<ALZUETA00>!
!***additions!
C6H6#+R1H=C6H7#                     3.2E13      0.0         3.2E3   !
<MEBEL97>!
C6H6#+B1O=C6H5O#+R1H                2.8E13      0.0        4.91E3   !
<EMDEE92>!
C6H6#+R2OH=C6H5OH#+R1H              1.3E13      0.0        10.6E3   !
<BAULCH94>!
C6H6#+R9C2H=C6H5#C2H+R1H            5.0E13      0.0           0.0   !
<WANG97>!
C6H6#+R10C2H3V=styrene+R1H          7.9E11      0.0         6.4E3   !
<WANG97>!
!***Metatheses!

!*modif Zhenyu*!
!C6H6#+R1H=C6H5#+H2                  6.0E8       1.8        16.8E3   !
<MEBEL97>!
C6H6#+R1H=C6H5#+H2                  1.22E8      2.031     15.88E3   !
calcul CBS-QB3 Fournet

C6H6#+B1O=C6H5#+R2OH              2.0E13    0.0        14.7E3   !
<LINDSTEDT94>!

!*modif Zhenyu*!
!C6H6#+R2OH=C6H5#+H2O                1.6E8       1.42       1.45E3   !
<BAULCH92>!
C6H6#+R2OH=C6H5#+H2O                  1.36E4      2.7      0.6196E3   !as
toluene+R2OH=C6H4CH3+H2O

!*modif Zhenyu*!
```

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!C6H6#+R3OOH=C6H5#+H2O2              5.5E12      0.0        28.9E3   !
<BAULCH94>!
C6H6#+R3OOH=C6H5#+H2O2               9.2E12      0.0       28.81E3   !as
toluene+R3OOH=C6H4CH3+H2O2

!*modif Zhenyu*!
!C6H6#+R4CH3=C6H5#+CH4                2.0E12      0.0        15.0E3   !
<ZHANG89>!
C6H6#+R4CH3=C6H5#+CH4                2.07E0      3.861      13.3E3   !
calcul CBS-QB3 Fournet

C6H6#+R11C2H5=C6H5#+C2H6             6.3E11      0.0        15.0E3   !
<ZHANG89>!
C6H5#+C3H6Y=C6H6#+C3H5Y              7.94E13     0.0       11.94E3   !MF
<Heckmann,Hippler,Troe(1996)>
C6H6#+nC4H5=C6H5#+C4H6Z2             6.3E11      0.0        15.0E3   !
estimated!
C6H6#+iC4H5=C6H5#+C4H6Z2             6.3E11      0.0        20.0E3   !
estimated!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=lC6H7                          2.5E14      0.7       41.8E3    !
<WEISSMAN89!

!***Decomposition by beta-scission!
!C6H7#=>C2H2+nC4H5                   2.0E13      0.0       50.0E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
HEYBERGER02!
!***Oxidation!
C6H7#+O2=C6H6#+R3OOH                 7.9E11      0.0        9.9E3    !
estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combimations!
C6H7#+R1H=C6H8#                      1.0E14      0.0        0.0      !
estimated!
!***Disproportionnations!
C6H7#+R1H=C6H6#+H2                   3.3E12      0.0        0.0      !
<RISTORI01>!
C6H7#+R2OH=C6H6#+H2O                 1.0E13      0.0        0.0      !
estimated!
C6H7#+R4CH3=C6H6#+CH4                3.0E12     -0.32      -0.1E3    !
estimated!
C6H7#+C6H7#=C6H6#+C6H8#              8.4E10      0.0       -0.3E3    !
estimated!
!analogy with the disproprotionnations ofC3H5Y proposed by TSANG91!

!REACTIONS OF C6H5# RADICALS!
!***Isomerization!
C6H5#=lC6H5                          5.0E13      0.0       72.5E3    !
<BRAUN89>!
!lC6H5 = ch///c/ch//ch/ch//ch(.)!
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lC6H5=>2C2H2+R9C2H                    2.0E13      0.0       51.0E3   !
estimated!
!DH298 =44kcal/mol, Eadd=7 kcal/mol!
lC6H5=lC6H4+R1H                          2.0E12      0.0
41.0E3   !estimated!
!lC6H4 = ch///c/ch//ch/c///ch , DH298 =38kcal/mol, Eadd=3 kcal/mol!
!from BRAUN89 at 1500 K!
!***Reactions with O2!
C6H5#+O2=C6H5O2                      2.2E19     -2.5         0.0    !
estimated!

C6H5#+O2=C6H5O#+B1O                  2.6E13      0.0         6.1E3    !
<FRANK94>!
C6H5#+O2=OC6H4O+R1H                  3.0E13      0.0         9.0E3    !
<FRANK94>!


!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!
!***Additions!
C6H5#+C2H2=C6H5#C2H+R1H              4.0E13      0.0        10.1E3    !
<MARINOV97>!
C6H5#+C6H6#=biphenyl+R1H             5.6E12     -0.074       7.5E3    !
<WANG97>!
!***Combinations!
C6H5#+B1O=C5H5#+B2CO                1.0E14      0.0           0.0     !
<FRANK94>!
C6H5#+R2OH=C6H5OH#                      1.0E13        0.0           0.0
!calculated!
!toluene=C6H5#+R4CH3                    1.0E16        0.0          97.0E3
!<COLKET94>!
!calculation by KINGAS!
C6H5#+R5CHO=C6H5CHO                  5.0E12      0.0         0.0      !
estimated!
C6H5#+R10C2H3V=styrene               5.0E12      0.0         0.0      !
estimated!
C6H5#+R11C2H5=etC6H5                 5.0E12      0.0         0.0      !
estimated!
C6H5#+R3OOH=C6H5O#+R2OH              5.0E12      0.0         0.0      !
estimated!
!C6H5C3H3 n'intervient qu'ici
!C6H5#+C3H3=C6H5C3H3                  3.0E12      0.0         0.0      !
<D'ANNA98>!
C6H5#+C6H5#=biphenyl                 3.8E31     -5.75        7.9E3    !
<WANG97>!
!***disproportionnations!
C6H5#+R2OH=C6H5O#+R1H                5.0E13      0.0         0.0      !
<ALZUETA00>!
C6H5#+C6H7#=C6H6#+C6H6#              1.0E12      0.0         0.0      !
<SHANDROSS96>!

!REACTIONS OF PHENYLPEROXY RADICALS!
!***Decomposition by beta-scission!
!mfC6H5O2=OC6H4O+R1H                     2.0E13      0.0        30.0E3    !
estimated!
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C6H5O2=C5H4O#+R5CHO                  2.0E13      0.0       30.0E3    !
estimated!
!see DA COSTA01!

!MF
C6H5O2+R3OOH=C6H5OOH+O2                    2.0E11          0.00  -1300
C6H5OOH=C6H5O#+R2OH                        1.5E16         0.00   43000


!REACTIONS OF PHENOXY RADICALS!
!***CO elimination!
C6H5O#=B2CO+C5H5#                    2.5E11      0.0      43.8E3    !
<BAULCH92>!
!***Combinations!
!--C6H5O#+R1H(+M)=C6H5OH#(+M)        2.5E14      0.0        0.0     !
<FRENKLACH>!
C6H5O#+R1H(+M)=C6H5OH#(+M)           1.0E14      0.0        0.0     !
estimated!
                           LOW   /1.0E94  -21.84   13.9E3/           !
<FRENKLACH>!
                           TROE /0.043 304 60000 5896/
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
C6H5O#+R1H=C5H6#+B2CO                1.1E53    -10.7        41.4E3   !
<TAN96>!
C6H5O#+B1O=OC6H4OH                   2.6E10      0.47        0.8E3   !
<LIN95>!
C6H5O#+B1O=OC6H4O+R1H                8.5E13      0.0         0.0     !
<FRANCK94>!
C6H5O#+B1O=C5H5#+CO2                 1.0E13      0.0         0.0     !
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!
!***CO elimination!
OC6H4OH=B2CO+C5H4OH#                 7.4E11      0.0        43.8E3   !
estimated!
!as for phenoxy radicals!

!REACTIONS OF CYCLOPENTADIENYL RADICALS!
!***Isomerization!
C5H5#=lC5H5                          1.0E14      0.0       45.5E3    !
<BRAUN89>!

!lC5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car lC5H6 n'intervient qu'ici
!lC5H5+R1H=lC5H6                     1.0E14      0.0        0.0      !
estimated!
lC5H5=C3H3+C2H2                     2.0E13      0.0        50.0E3   !
estimated!
!DH298 =43kcal/mol, Eadd=7 kcal/mol!


!***Reactions with O2!
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```
C5H5#+O2=R5CHO+C4H4O                  1.2E19     -2.48      11.0E3    !
<ZHONG98>!
!***Combinations!
C5H6# = C5H5# + R1H                          5.0E15          0.00   7.87E4
     ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>

C5H5#+B1O=C5H4O#+R1H                  5.8E13     -0.02       0.02E3   !
<ZHONG98>!
C5H5#+B1O=>2C2H2+R5CHO                3.2E13     -0.17       0.44E3   !
<ZHONG98>!
C5H5#+R2OH=>C4H6Z2+B2CO                4e14       0.0         4500 !
[PENGLOAN- RODA]


C5H5#+R2OH=C5H5OH#                   1.0E13      0.0         0.0      !
calculated!
C5H5#+R3OOH=C5H5O#+R2OH               3.0E12      0.0         0.0      !
calculated!
!calculation by KINGAS!
C5H5#+C5H5#=>C10H10#                  2.0E12      0.0         0.0      !
estimated!
C10H10#=>C5H5#+C5H5#                  3.2E15      0.0         57.5E3   !
calculated!
!***disproportionnations!
C5H5#+R3OOH=>C5H6#+O2                 2.5E9       1.0         3.5E3    !
estimated!
!estimated as for allylic radicals (HEYBERGER02)/10!

!REACTIONS OF CYCLOPENTADIONYL RADICALS!
!***Decompositions by beta-scission!
C5H5O#=>2C2H2+R5CHO                    2.0E13      0.0        30.0E3   !
estimated!
C5H5O#=C5H4O#+R1H                     2.0E13      0.0         30.0E3   !
estimated!
!see DA COSTA01!
!***Combinations!
C5H5O#+R1H=C5H5OH#                    1.0E14      0.0         0.0      !
estimated!
!***no disproportionnations considered!

!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!
C5H4OH#+O2=C5H4O#+R3OOH               1.0E13      0.0         5.0E3    !
estimated!
C5H4OH#+R1H=C5H5OH#                   1.0E14      0.0         0.0      !
estimated!
C5H4OH#+B1O=CO2+C2H2+R10C2H3V         3.2E13     -0.17        0.44E3   !
estimated!
!C5H4OH#+R3OOH=>R2OH+CO2+R10C2H3V+C2H2 3.0E12      0.0         0.0      !
estimated!
C5H4OH#+R3OOH=>R2OH+R2OH+C5H4O# 3.0E12      0.0         0.0      ! mf

C5H4OH#+R3OOH=>C5H5OH#+O2             2.5E9       1.0         3.5E3    !
estimated!
!Reactions derived from those of cyclopentadienyl radicals!
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C5H4OH#+C6H5O#=C5H4O#+C6H5OH#        1.0E12      0.0        0.0      !
estimated!


!
*********************************************************************
*********!
!*
!*                    SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!*
!
*********************************************************************
*********!

!REACTIONS OF ORTHOBENZOQUINONE!
OC6H4O=>C5H4O#+B2CO                  1.0E12      0.0       40.0E3    !
<ALZUETA00>!
OC6H4O+R1H=>2B2CO+C2H2+R10C2H3V      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
!OC6H4O+R1H=>H2+2B2CO+C2H2+R9C2H      1.6E6       2.5        9.8E3    !
estimated!
!OC6H4O+R2OH=>H2O+2B2CO+C2H2+R9C2H    4.4E6       2.0        1.4E3    !
estimated!
!estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!
C6H5OH#=C5H6#+B2CO                   1.0E12      0.0        61.2E3   !
<HORN98>!


C6H5OH#+O2=R3OOH+C6H5O#              1.0E13     0.0       38.9E3    !
<ALZUETA00>!


C6H5OH#+B1O=OC6H4OH+R1H              1.6E13     0.0         3.4E3    !
estimated!


!as the addition of O-atoms to toluene (DACOSTA01)!
C6H5OH#+R1H=C6H5O#+H2                1.2E14     0.0       12.4E3    !
<ALZUETA00>!
C6H5OH#+B1O=C6H5O#+R2OH              1.3E13     0.0        2.9E3  !
<ALZUETA00>!
C6H5OH#+R2OH=C6H5O#+H2O              1.4E8      1.4       -0.96E3  !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H5O#+H2O2            1.0E12      0.0       10.0E3    !
<ALZUETA00>!
C6H5OH#+R4CH3=C6H5O#+CH4             1.8E11      0.0        7.7E3    !
<MULCAHY65>!
C6H5OH#+C6H5#=C6H5O#+C6H6#           4.9E12      0.0        4.4E3    !
<ALZUETA00>!
!C6H5OH#+C5H5#=C6H5O#+C5H6#          4.9E11         0.0        9.4E3    !
estimated!
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!C6H5OH#+C3H5Y=C6H5O#+C3H6Y          4.9E11     0.0        9.4E3    !
estimated!
!C6H5OH#+iC4H5=C6H5O#+C4H6Z2          4.9E11          0.0        9.4E3    !
estimated!
C6H5OH#+C5H5#=C6H5O#+C5H6#           2.67e14          0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+C3H5Y=C6H5O#+C3H6Y          2.67e14     0.0        25.238e3    !mf
<Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+iC4H5=C6H5O#+C4H6Z2          2.67e14          0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>


!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!
C6H5OH#+R1H=C6H4OH#+H2               1.7E14      0.0        16.0E3    !
<SHANDROSS96>!
C6H5OH#+B1O=C6H4OH#+R2OH             2.0E13     0.0          14.7E3    !
estimated!
C6H5OH#+R2OH=C6H4OH#+H2O             1.4E13     0.0        4.6E3   !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H4OH#+H2O2           4.0E11      0.0        28.9E3    !
estimated!
C6H5OH#+R4CH3=C6H4OH#+CH4           2.0E12      0.0        15.0E3    !
estimated!
!as the H-abstractions from benzene!

C6H4OH#+O2=OC6H4OH+B1O               2.1E13      0.0        6.1E3    !
estimated!
!as for phenyl radicals (FRANCK94)!
C6H4OH#+R1H=C6H5OH#                  1.0E14      0.0        0.0      !
estimated!
C6H4OH#+R4CH3=HOC6H4CH3              5.0E12      0.0        0.0      !mf


!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!
C5H6#+O2=>C5H5#+R3OOH                1.4E12      0.0        31.6E3   !
<INGHAM94>!
!C5H6#+R1H=C5H7#                      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
C5H6#+B1O=>C5H5O#+R1H                8.9E12     -0.15       590.0    !
<ZHONG98>!
C5H6#+R1H=C5H5#+H2                   2.8E13      0.0        2.0E3    !
<ROY97>!
C5H6#+B1O=C5H5#+R2OH                 4.8E4       2.7        1.1E3    !
<ZHONG98>!
C5H6#+R2OH=C5H5#+H2O                 3.1E6       2.0        0.0      !
<ZHONG98>!
C5H6#+R3OOH=C5H5#+H2O2               1.1E4       2.6        12.9E3    !
<ZHONG98>!
C5H6#+R4CH3=C5H5#+CH4                1.8E-1      4.0        0.0      !
<ZHONG98>!
C5H6#+C3H5Y=C5H5#+C3H6Y             1.6E12        0.0      15.1E3    !
astoluene!
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C5H6#+nC4H5=C5H5#+C4H6Z2            1.6E12       0.0      11.1E3    !
astoluene!
C5H6#+iC4H5=C5H5#+C4H6Z2            1.6E12       0.0      15.1E3    !
astoluene!
!C5H6#+C3H5Y=C5H5#+C3H6Y            6.0E12      0.0        0.0      !
estimated!
!C5H6#+nC4H5=C5H5#+C4H6Z2            6.0E12      0.0        0.0      !
estimated!
!C5H6#+iC4H5=C5H5#+C4H6Z2            6.0E12      0.0        0.0      !
<EMDEE92>!

!C5H7#=>C2H2+C3H5Y                   2.0E13      0.0       35.5E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by
HEYBERGER02!
!C5H7#+O2=C5H6#+R3OOH                7.9E11      0.0        5.0E3    !
estimated!
!oxidation of an alkylic radical!

!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!
C5H4O#=>2C2H2+B2CO                    5.7E32     -6.76      68.5E3    !
<ALZUETA00>!
!C5H4O#=B2CO+C4H4                     1.00e12     0.0        53000    !
roda PENGLOAN!
C5H4O#+R1H=B2CO+nC4H5                2.6E13      0.0        3.2E3    !
estimated!


!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!
C5H4O#+B1O=C4H4+CO2                  1.0E13     0.0        2.0E3     !
<ALZUETA00>!
C5H4O#+R1H=C5H3O#+H2                 8.13E7     2.031    15.88E3     !MF
idem C6H6#+R1H=C6H5#+H2
C5H4O#+B1O=C5H3O#+R2OH               1.4E13     0.0       14.7E3     !
<ALZUETA00>!
C5H4O#+R2OH=C5H3O#+H2O               1.1E8      1.42       1.4E3     !
<ALZUETA00>!

C5H3O#=>C2H2+B2CO+R9C2H               2.0E13     0.0        51.0E3    !
estimated!
!estimated as the decomposition of lC6H5!
C5H3O#+O2=>CO2+C2H2+R12CHCOZ          9.7E58   -13.47       38.2E3    !
<ALZUETA00>!

C5H5OH#+R1H=C5H5O#+H2              4.0E13      0.0        6.1E3    !
<ALZUETA00>!
C5H5OH#+B1O=C5H5O#+R2OH              1.0E13      0.0        4.6E3    !
<ALZUETA00>!
C5H5OH#+R2OH=C5H5O#+H2O              1.0E13      0.0        1.7E3    !
<ALZUETA00>!

!Estimated from the same reaction for CH3OH!
```

```
C5H5OH#+R1H=C5H4OH#+H2                  1.4E13      0.0       2.0E3    !
estimated!
C5H5OH#+B1O=C5H4OH#+R2OH              4.8E4      2.7        1.1E3    !
estimated!
C5H5OH#+R2OH=C5H4OH#+H2O              1.5E6      2.0        0.0E3    !
estimated!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!
!additions decomposition
C4H4O+R1H=>R10C2H3V+CH2COZ             1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>C2H4Z+R12CHCOZ              1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>sC3H5+B2CO                  1.3E13    0.0        1.5E3     !
estimated!
C4H4O+R2OH=>C2H3CHO+R5CHO              1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+R2OH=>CO2+C3H5Y                 1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+B1O=>R13CH2CHO+R12CHCOZ          6.0E4     2.56      -1.1E3     !
estimated!
C4H4O+B1O=>2CH2COZ                     6.0E4     2.56      -1.1E3     !
estimated!
!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition
C4H4O+R1H=>C2H2+R12CHCOZ+H2            8.2E5     2.5        12.3E3    !
estimated!
C4H4O+R1H=>C3H3+B2CO+H2                4.1E5     2.5         9.8E3    !
estimated!
C4H4O+R2OH=>C2H2+R12CHCOZ+H2O          2.2E6     2.0         2.8E3    !
estimated!
C4H4O+R2OH=>C3H3+B2CO+H2O              1.1E6     2.0         1.5E3    !
estimated!
C4H4O+B1O=>C2H2+R12CHCOZ+R2OH          1.2E11    0.7         8.7E3    !
estimated!
C4H4O+B1O=>C3H3+B2CO+R2OH              6.0E10    0.7         8.7E3    !
estimated!
!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!


!
*************************************************************************
*********!
!*                                                          *!
!*             MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE
*!
!*                                                          *!
!*    efficiency  coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#
and toluene*!
!*                                                          *!
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!
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*********!
!*                                                          *!
!*            PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE
*!
!*                                                          *!
!
*********************************************************************
*********!

!*********************************!
!*REACTIONS OF TOLUENE MOLECULES*!
!*********************************!

!**UMIMOLECULAR INITITIATIONS


toluene=benzyl+R1H              2.09E15  0.0   87.51E3    !
<Oehlschlaeger07>! Zhenyu
toluene=C6H5#+R4CH3               2.66E16  0.0   97.88E3    !
<Oehlschlaeger07> Zhenyu

!**BIMOLECULAR INITITIATION
toluene+O2=benzyl+R3OOH      1.8E12   0.0    39.7E3    !<BAULCH94>!
!toluene+O2=benzyl+R3OOH      2.18e7   2.50    46045    !
mf<Oehlschlaeger06>!

!**ADDITIONS

toluene+R1H=C6H6#+R4CH3           5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet Zhenyu

toluene+B1O=OC6H4CH3+R1H      1.7E13   0.0     3.6E3    !<TAPPE89>!
!toluene+R2OH=HOC6H4CH3+R1H         2.3E12   0.0   -0.36E3   !<BAULCH92>!
toluene+R2OH=HOC6H4CH3+R1H    1.3E13   0.0    10.6E3    !<BAULCH94>as
benzene!

toluene+R2OH=C6H5OH#+R4CH3     7.83E2   2.884  3.2193E3  !Seta V Nakajima
V Miyoshi JPCA 2006 Zhenyu
!toluene+R2OH=C6H5OH#+R4CH3     1E5    2.58   1134.0    !Olive as
benzene+OH


!**METATHESES
!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

toluene+R1H=benzyl+H2         2.92E6   2.372  5.81E3   !Calcul CBS-QB3
Fournet Zhenyu
```

```
toluene+B1O=benzyl+R2OH            6.3E11   0.0       0.0   !
<HOFFMANN90>!

toluene+R2OH=benzyl+H2O            5.2E09   1.0    0.87E3   !<BAULCH94>!

toluene+R3OOH=benzyl+H2O2     4.0E11   0.0    14.0E3   !<BAULCH94>!
toluene+R4CH3=benzyl+CH4      3.91E0   3.76   6.98E3   !Calcul CBS-QB3
Fournet Zhenyu

! ajout MF
toluene+R7CH3O=benzyl+CH3OH     2.12E+10 0.0 3000.0        !PITZ2001
toluene+R8CH3OO=benzyl+CH3OOH   1.02E+04 2.5 12339.3  !PITZ2001


!toluene+R5CHO=benzyl+HCHO     3.77E13   0.0 23.7874E3    !MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO           1.26e8   1.9   18.183E3
benzyl+CH3CHO = toluene+R14CH3CO 1.26e8   1.9   18.183E3

toluene+R10C2H3V=benzyl+C2H4Z  4.0e12   0.0     8.0e3       !<COLKET94>!

toluene+C3H5Y=benzyl+C3H6Y    1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+C3H3=benzyl+pC3H4     1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2         1.6E12   0.0    15.1E3   !
<estimated(a)>!
toluene+nC4H5=benzyl+C4H6Z2         1.6E12   0.0    11.1E3   !
<estimated(a)>!
toluene+C5H5#=benzyl+C5H6#    1.6E11   0.0    15.1E3   !<estimated(a)>!
!(a) :Rate constant taken equal to that of the H-abstraction with methyl
radicals proposed !
!by COLKETT94 with A divided by 10 for cyclic radicals !
! and with an activation energy 4 kcal/mol higher for resonnance
stabilised radicals!



!ajout MF
toluene+C6H5O2=benzyl+C6H5OOH                 1.02E+04 2.5 12339.3    !
PITZ2001


toluene+C6H5#=benzyl+C6H6#    7.9E13   0.0    12.0E3   !<HECKMANN96>!

toluene+C6H5O#=benzyl+C6H5OH#         1.6E11   0.0   15.1E3 !
<estimated(a)>! peut etre trop rapide
toluene+C6H4CH3=benzyl+toluene       7.9E13   0.0   12.0E3  !
<estimated(b)>!
toluene+OC6H4CH3=benzyl+HOC6H4CH3   1.6E11   0.0   15.1E3  !
<estimated(a)>!
toluene+C6H5CH2OO=benzyl+C6H5CH2OOH 4.0E11   0.0   14.0E3  !
<estimated(c)>!
toluene+C6H5CH2O=benzyl+C6H5CH2OH     1.6E11   0.0   11.1E3 !
<estimated(a)>!
toluene+HOC6H4CH2=benzyl+HOC6H4CH3  1.6E11   0.0   15.1E3  !
<estimated(a)>!
```

```
!(b) :Rate constant taken equal to that of the H-abstraction with phenyl
radicals proposed !
!by HECKMANN96!
!(c) :Rate constant taken equal to that of the H-abstraction with HO2
radicals proposed !
!by BAULCH94!

!**METATHESES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2          1.22E08  2.031 15.88E3  !as
C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu
toluene+B1O=C6H4CH3+R2OH   2.0E13   0.0    14.7E3     !<estimated(d)>!

toluene+R2OH=C6H4CH3+H2O     1.36E4   2.7  0.6196E3   !<Seta06>! in
Sakai07 Zhenyu
toluene+R3OOH=C6H4CH3+H2O2   9.2E12   0.0   28.81E3   !<Baulch94>! in
Sakai07 Zhenyu
toluene+R4CH3=C6H4CH3+CH4   2.07E0   3.861  13.3E3    !as
C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu


!******************************!
!*REACTIONS OF BENZYL RADICALS*!
!******************************!

!**DECOMPOSITION BY BETA-SCISSION
benzyl=>C5H5#+C2H2             6.0E13   0.0    70.0E3 !<Colket94>!
benzyl=>C3H3+C4H4              2.0E14   0.0    83.6E3 !<Colket94>!

!**REACTIONS WITH OXYGEN
benzyl+O2=C6H5CH2OO                4.6E11   0.0   -377.0   !<FENTER94>!
benzyl+O2=C6H5CH2O+B1O         6.3E12   0.0   40.0E3  !<BREZYNSKY84>!

!**TERMINATION REACTIONS
benzyl+B1O=C6H5#+HCHO         3.5E13   0.0      0.0   !<EMDEE92>!
benzyl+B1O=C6H5CHO+R1H              1.0E14   0.0      0.0   !
<estimated(e)>!
!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4
!(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH3OO=>C6H5CH2O+R7CH3O            5.0E12     0.0        0.0
benzyl+R17C2H5OO=>C6H5CH2O+R15C2H5O        5.0E12     0.0        0.0

benzyl+R2OH=C6H5CH2OH          2.0E13   0.0      0.0  !<HIPLER91>!

!MFbenzyl+R3OOH=C6H5CH2OOH        5.0E12   0.0      0.0    !<HIPPLER92>!
benzyl+R3OOH=C6H5CH2OOH           8.21E4   2.20      -5.13E3     !MF<da
silva-bozzelli- proceedings  comb inst 32(2009)287-294>!

2benzyl=bibenzyl                    5.01E12   0.0 0.454E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3           6.1e15    0.0   75120   !<BAULCH94>!
```

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!************************************!
!*REACTIONS OF METHYL PHENYL RADICALS*!
!************************************!

!**reactions with oxygen
!mfC6H4CH3+O2=OC6H4CH3+B1O                  2.6E13   0.0   6.1E3  !
<estimated(f)>!
!mfC6H4CH3+O2=OC6H4O+R4CH3                  3.0E13   0.0   9.0E3  !
<estimated(f)>!
!(f) : Rate constant taken equal to that of the similar reaction in the
case of phenyl!
!radicals!

!ajout mf
C6H4CH3+O2=>OOC6H4CH3                 3.72E13         -0.22      -711
     !2008DAS/BOZ3566-3575
OOC6H4CH3=>C6H4CH3+O2                 6.36E19        -1.372     48.74E3
          !2008DAS/BOZ3566-3575
OOC6H4CH3=>OC6H4CH3+B1O                     1.27E15         -0.25
     3.85E4          !2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3                     5.0E11          0.00
     46400      !



!***termination reactions!
C6H4CH3+R1H=toluene                   1.0E14   0.0   0.0    !
<estimated(g)>!
!(g) : Rate constant taken equal to that of the recombination of H atoms
with alkyl !
!radicals as proposed by Allara!


C6H4CH3+B1O=OC6H4CH3                  1.0E14   0.0   0.0    !
<estimated(f)>!
C6H4CH3+R2OH=HOC6H4CH3                1.0E13   0.0    0.0   !
<estimated(f)>!
C6H4CH3+R4CH3=C8H10#            1.2E06   1.96   -3.7E3     !
<estimation(fbis)>!
!(fbis) : Rate constant taken equal to that of the similar reaction in
the case of phenyl!
!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH           5.0E12   0.0   0.0    !
<estimated(f)>!
C6H4CH3 +R1H = benzyl + R1H           1.0E13   0.0   0.0    !<MILLER92>!

!************************************!
!*REACTIONS OF BENZYL PEROXY RADICALS*!
!************************************!


!**isomerisation-decomposition reactions
```

```
C6H5CH2OO=C6H5CHO+R2OH                      3.4E9   1.0   37.5E3  !
<estimated(h)>!
!(h) : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 23 (4 membered transition
ring)!
!+ 14.5 (secondary allylic H-atom)!

!**Combination reactions
!MF C6H5CH2OO+R1H=C6H5CH2OOH               1.0E14   0.0   0.0E3  !
<estimated(g)>!

!**dispropotionnation reactions!
C6H5CH2OO+R3OOH=C6H5CH2OOH+O2         2.0E11   0.0   -1.3E3 !
<estimated(i)>!
2C6H5CH2OO=C6H5CH2OH+C6H5CHO+O2       1.4E10   0.0   -725.0 !
<estimated(i)>!
C6H5CH2OO+C6H5CH2OO=2C6H5CH2O+O2      6.3E10   0.0   -725.0 !
<estimated(i)>!
!(i) : Rate constant taken equal to that the disproportionnation of
peroxyalkyl radicals !
!as proposed by Warth!


! ajout MF
C6H5CH2OO+R1H=C6H5CH2O+R2OH                      3.80E14         -0.19
     1.89E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=C6H5CH2OOH              4.35e60         -15.92     11.40E3
     !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=benzyl+R3OOH                  1.96E4          2.47  1.43E3
     !<da silva J Chem Theory Comput 2009>


!************************************!
!*REACTIONS OF BENZYL ALCOXY RADICALS*!
!************************************!

!**Decomposition by beta-scission ************
C6H5CH2O=R1H+C6H5CHO                        2.0E13   0.0   27.5E3 !
<estimated(j)>! INHIBE
C6H5CH2O=C6H5#+HCHO                         2.0E13   0.0   27.5E3 !
<estimated(j)>! ACCELERE
!DH = 23.59 kcal/mol!
!(j) For these beta-scissions involving the breaking of a C-C or a C-H
bond,  A-factor !
!is an average value for beta-scissions [Heyberger] and activation
energies have been!
! estimated from thermochemistry and to obtain the best results!

!C6H5CH2O=R1H+C6H5CHO                       5.26E28   -5.081   22.25E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H6#+R5CHO                       2.37E32   -6.095   28.81E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H5#+HCHO                        7.21E33   -6.21    36.85E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
```

```
!C6H5CH2O=R1H+C6H5CHO                          1.00e14   0.00   2.91e4    !
mf<Mehl Proc comb inst 33(2011)193>!
!C6H5CH2O=C6H5#+HCHO                           1.46e20   -2.00  3.51e4    !
mf<Mehl Proc comb inst 33(2011)193>!



!***reactions with oxygen
C6H5CH2O+O2=R3OOH+C6H5CHO                      6.0E10   0.0   1.6E3  !
<estimated(k)>!
!(k) : Rate constant taken equal to that of the similar reaction in the
case of ethoxy!
!radicals as proposed by BAULCH92!

!*******************************!
!*REACTIONS OF CRESOXY RADICALS*!
!*******************************!

!**OC6H4CH3=HOC6H4CH2           2.9E9   1.0   3.2E3   !<estimated(h')>!
!(h') : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 5.9 + 5 (5 membered
transition ring)!
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2             1.1E9   1.0   22.9E3  !
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by ROO.
close bde)

!**CO elimination with rearrangement
!OC6H4CH3=>R1H+C6H6#+B2CO                 7.5E11  0.0  43.8E3 !
<FRANCK94>!
OC6H4CH3=>R1H+C6H6#+B2CO                3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>R10C2H3V+C4H4+B2CO            3.0E11  0.0  43.8E3!<FRANCK94>!
!OC6H4CH3=>C2H2+iC4H5+B2CO               3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO            3.0E11  0.0  43.8E3    !
<FRANCK94>!
OC6H4CH3=>C3H3+aC3H4+B2CO                1.5E11  0.0  43.8E3     !
<FRANCK94>!

!**termination reactions!
OC6H4CH3+R1H=HOC6H4CH3                1.0E14   0.0   0.0E3  !
<estimated(g)>!

!
*************************************************************************
*********!
!*
                                          *!
!*                    SECONDARY MECHANISM OF THE OXIDATION OF TOLUENE
            *!
```

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!*                                                                    *!
!
!*********************************************************************
*********!

!************************************************!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!************************************************!

! Amorcage
!C6H5CHO+O2=C6H5CO+R3OOH         2.0E13   0.0   38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R3OOH          7.0E11   0.0   39.5E3 !RODA RODA
C6H5CHO = C6H5CO + R1H    3.98E15 0.0 83.74E3  !NIST GRELA86!

! Addition
C6H5CHO+R1H=C6H6#+R5CHO          5.8E13   0.0   8.1E3       !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13     0.0        3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the  resonnance
stabilisation of the!
! obtained radical!

C6H5CHO+B1O=C6H5CO+R2OH          6.0E12     0.0   1.8E3 !<BAULCH94>!
C6H5CHO+R2OH=C6H5CO+H2O          7.8E12     0.0   0.0   !<BAULCH94>!
C6H5CHO+R3OOH=C6H5CO+H2O2  3.0E12     0.0   11.0E3     !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4   2.0E-6     5.6   2.5E3 !MF <BAULCH94>!

C6H5CHO+R11C2H5=C6H5CO+C2H6      1.3E12     0.0   7.5E3 !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the  !
!resonnance stabilisation of the obtained radical!

C6H5CHO+C3H5Y=C6H5CO+C3H6Y 1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2      1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+nC4H5=C6H5CO+C4H6Z2      1.3E12         0.0           7.5E3      !
<estimated(p)>!
C6H5CHO+benzyl=toluene+C6H5CO         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5O#=C6H5CO+C6H5OH#         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+OC6H4CH3=C6H5CO+HOC6H4CH3     1.3E11     0.0   11.5E3     !
<estimated(p)>
```

```
C6H5CHO+C5H5#=C6H5CO+C5H6#      1.3E11     0.0   11.5E3     !
<estimated(p)>
!(p) :Rate constant taken equal to that of the H-abstraction with ethyl
radicals  !
! with A divided by 10 for cyclic radicals and with an activation
energy !
!4 kcal/mol higher for resonnance stabilised radicals!

C6H5CHO+HOC6H4CH2=C6H5CO+HOC6H4CH3    1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5#=C6H5CO+C6H6#      1.3E11     0.0   11.5E3   !<estimated(p)>

C6H5CO=C6H5#+B2CO                        4E14   0.0      29.5e3   !
<SOLLY71>!
!Author(s):   Solly, R.K.; Benson, S.W.
!Title:   Kinetics of the gas-phase unimolecular decomposition of the
benzoyl radical
!Journal:   J. Am. Chem. Soc.
!Volume:   93
!Page(s):   2127
!Year:   1971

!***********************************!
!*REACTIONS OF BENZYL HYDROPEROXYDE*!
!***********************************!

!MFC6H5CH2OOH=C6H5CH2O+R2OH           1.5E16     0.0   42.0E3     !
<estimated(r)>!
!(r) : Rate constant taken equal to that the decomposition of
hydroperoxide species !
! proposed by Bounaceur <SAHETCHIAN>!
!MFC6H5CH2OOH=C6H5CH2O+R2OH           2.03E47         -10.27
     50.71E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OOH=C6H5CH2O+R2OH        3.29E13         0.42       39.89E3  !
MF<da silva Proc comb inst 32(2009)287-294>
C6H5CH2OOH=C6H5CHO+H2O                7.45E8          1.19
     46.04E3  !MF<da silva Proc comb inst 32(2009)287-294>


!****************************************!
!*REACTIONS OF CRESOL AND DERIVED RADICALS*!
!****************************************!

! amorcage
HOC6H4CH3+O2=OC6H4CH3+R3OOH           1.0E13     0.0   38.9E3     !
<estimated(s)>! ralenti
!A=1E13 pour phenol!
!(s) : Rate constant taken equal to that of the same reaction for
phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R3OOH         2.1E13      0.0       38.0E3    !
<EMDEE92*2>!
HOC6H4CH3+O2=HOC6H4CH2+R3OOH          2.1E12      0.0       38.6E3    !
RODA <estimated(aaa)>!
```

```
! addition
HOC6H4CH3+R1H=C6H5OH#+R4CH3              5.8E13      0.0          8.1E3
!<estimated(t)>!
!(t) : Rate constant taken equal to that of the same reaction for toluene
!

!HOC6H4CH2+B1O=C6H4OH#+HCHO 8E13 0.0 0.0




! metatheses
HOC6H4CH3+R1H=OC6H4CH3+H2          1.2E14  0.0   12.4E3     !
<estimated(s)>!
HOC6H4CH3+B1O=OC6H4CH3+R2OH              1.3E13  0.0   2.9E3 !
<estimated(s)>!
HOC6H4CH3+R2OH=OC6H4CH3+H2O           1.4E8 1.4   -0.96E3    !
<estimated(s)>!
HOC6H4CH3+R3OOH=OC6H4CH3+H2O2         1.0E12     0.0   10.0E3     !
<estimated(s)>!
HOC6H4CH3+R4CH3=OC6H4CH3+CH4          1.8E11     0.0   7.7E3 !
<estimated(s)>!
HOC6H4CH3+C6H5#=OC6H4CH3+C6H6#        4.9E12     0.0   4.4E3 !
<estimated(s)>!
HOC6H4CH3+C5H5#=OC6H4CH3+C5H6#        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2       4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH#     4.9E11     0.0   9.4E3   !
<estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2         1.2E14      0.0       8.4E3   !
<estimated(t)>!
HOC6H4CH3+B1O=HOC6H4CH2+R2OH          6.3E11        0.0
0.0     !<estimated(t)>!
HOC6H4CH3+R2OH=HOC6H4CH2+H2O          5.2E9       1.0       0.87E3  !
<estimated(t)>!
HOC6H4CH3+R3OOH=HOC6H4CH2+H2O2        4.0E11      0.0       14.0E3  !
<estimated(t)>!
HOC6H4CH3+R4CH3=HOC6H4CH2+CH4         1.6E12        0.0       11.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H5Y=HOC6H4CH2+C3H6Y 1.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H3=HOC6H4CH2+pC3H4        1.6E12        0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+iC4H5=HOC6H4CH2+C4H6Z21.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+nC4H5=HOC6H4CH2+C4H6Z2      1.6E12        0.0       11.1E3  !
<estimated(t)>!
```

```
HOC6H4CH3+C5H5#=HOC6H4CH2+C5H6# 1.6E11         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C6H5#=HOC6H4CH2+C6H6# 7.9E13      0.0       12.0E3    !
<estimated(t)>!
HOC6H4CH3+C6H5O#=HOC6H4CH2+C6H5OH#    1.6E11         0.0       15.1E3   !
<estimated(t)>!
HOC6H4CH3+C6H4CH3=HOC6H4CH2+toluene   7.9E13      0.0       12.0E3   !
<estimated(t)>!
HOC6H4CH3+OC6H4CH3=HOC6H4CH2+HOC6H4CH3          1.6E11     0.0
15.1E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2OO=HOC6H4CH2+C6H5CH2OOH   4.0E11     0.0
14.0E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2O=HOC6H4CH2+C6H5CH2OH          1.6E11     0.0
11.1E3   !<estimated(t)>!

HOC6H4CH2+O2=HOC6H4CH2OO              4.6E11     0.0   -377.0     !
<estimated(u)>!
HOC6H4CH2+O2=HOC6H4CH2O+B1O           6.3E12     0.0   40.0E3     !
<estimated(u)>!
HOC6H4CH2+R3OOH=HOC6H4CH2O+R2OH       5.0E12     0.0   0.0   !
<estimated(u)>!
!(u) : Rate constant taken equal to that of the same reaction for benzyl
radicals !

HOC6H4CH2+R1H=HOC6H4CH3               1.0E14     0.0   0.0   !
<estimated(g)>!
HOC6H4CH2+R4CH3=C6H5OH#+C2H4Z         5.0E12     0.0   0.0   !
<estimated(g)>!

HOC6H4CH2OO=C6H4OHCHO+R2OH      3.4E9 1.0   37.5E3     !<estimated(v)>!
!(v) : Rate constant taken equal to that of the same reaction for benzyl
peroxy radicals !

HOC6H4CH2O=R1H+C6H4OHCHO              2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O=C6H4OH#+HCHO               2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O+O2=R3OOH+C6H4OHCHO         6.0E10      0.0       1.6E3     !
<estimated(w)>!
!(w) : Rate constant taken equal to that of the same reaction for benzyl
alcoxy radicals !

C6H4OHCHO+R1H=C6H4OHCO+H2       4.0E13     0.0   3.2E3 !<estimated(x)>!
C6H4OHCHO+B1O=C6H4OHCO+R2OH           6.0E12     0.0   1.8E3 !
<estimated(x)>!
C6H4OHCHO+R2OH=C6H4OHCO+H2O           7.8E12     0.0   0.0   !
<estimated(x)>!
C6H4OHCHO+R3OOH=C6H4OHCO+H2O2         3.0E12     0.0   11.0E3     !
<estimated(x)>!
C6H4OHCHO+R4CH3=C6H4OHCO+CH4          2.0E-6     5.6   1.5E3 !
<estimated(x)>!
!(x) : Rate constant taken equal to that of the same reaction for
benzaldehyde !
```

```
C6H4OHCO=C6H4OH#+B2CO                2.0E13 0.0   30.5E3     !
<estimated(y)>
!(y) : Rate constant taken equal to that of the same reaction for C6H5CO
radicals !

!************************************************!
!*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS*!
!************************************************!

C6H5CH2OH+O2=R3OOH+C6H5CHOH           1.4E12     0.0   34.0E3    !RODA
<estimated(aaa)>!
C6H5CH2OH+O2=C6H5CH2O+R3OOH           2.0E14     0.0   41.4E3    !
<EMDEE92>!

C6H5CH2OH+R1H=C6H6#+R6CH2OH           5.8E13  0.0     8.1E3     !
<estimated(t)>!

C6H5CH2OH+R1H=C6H5CHOH+H2        8.0E13     0.0   6.4E3 !<estimated(t')>!
C6H5CH2OH+B1O=C6H5CHOH+R2OH           4.2E11     0.0    -2.0E3   !
<estimated(t')>!
C6H5CH2OH+R2OH=C6H5CHOH+H2O           3.5E9 1.0    -1.13E3  !
<estimated(t')>!
C6H5CH2OH+R3OOH=C6H5CHOH+H2O2         2.7E11     0.0   12.0E3     !
<estimated(t')>!
C6H5CH2OH+R4CH3=C6H5CHOH+CH4          1.1E12     0.0   9.1E3 !
<estimated(t')>!
C6H5CH2OH+C3H5Y=C6H5CHOH+C3H6Y          1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+iC4H5=C6H5CHOH+C4H6Z2         1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+nC4H5=C6H5CHOH+C4H6Z2         1.112    0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C6H5#=C6H5CHOH+C6H6#        5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H4CH3=C6H5CHOH+toluene    5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H5O#=C6H5CHOH+C6H5OH#       1.1E11   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+benzyl=C6H5CHOH+toluene     1.1E11     0.0   13.1E3     !
<estimated(t')>!
C6H5CH2OH+OC6H4CH3=C6H5CHOH+HOC6H4CH3 1.1E11     0.0   13.1E3     !
<estimated(t')>!
C6H5CH2OH+HOC6H4CH2=C6H5CHOH+HOC6H4CH3     1.1E11     0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C5H5#=C6H5CHOH+C5H6#        1.1E11     0.0   13.1E3  !
<estimated(t')>!
!t': estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H                    2.0E13     0.     36.373E3    !MF
DHr=36.79 correlation baptiste E=0.6*DHr+14.3
!R15C2H5O=CH3CHO+R1H                2.0E14     0.     23.3E3 !(243,-
243)<HEICKLEN88NIST>!
```

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!************************************************!
!*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS*!
!************************************************!

!** Amorзages monomolйculaires
etC6H5 = R1H + C8H9#     4.3E14 0.0 83.6E3   !<kingas>!

!** Amorзages bimolйculaires
etC6H5+O2=C8H9#+R3OOH             1.4E12   0.0   34.0E3    !
<estimated(aaa)>!
etC6H5+O2=C8H9#-1+R3OOH           1.2E13        0.0     49.0E3    !
<exgas>!

!** Additions ipso
etC6H5+R1H=C6H6#+R11C2H5           5.8E13       0.0   8.1E3    !
<estimated(t)>!

!** Metatheses
etC6H5+R1H=C8H9#+H2                   8.0E13     0.0        6.4E3
     !<estimated(t")>!
etC6H5+B1O=C8H9#+R2OH           4.2E11     0.0    -2.0                !
<estimated(t")>!
etC6H5+R2OH=C8H9#+H2O           3.5E9 1.0    -1.13E3        !
<estimated(t")>!
etC6H5+R3OOH=C8H9#+H2O2               2.7E11     0.0        12.0E3
     !<estimated(t")>!
etC6H5+R4CH3=C8H9#+CH4             1.1E12  0.0        9.1E3           !
<estimated(t")>!
etC6H5+C3H5Y=C8H9#+C3H6Y        1.1E12     0.0        13.1E3          !
<estimated(t")>!
etC6H5+iC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+nC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+C6H5O#=C8H9#+C6H5OH#     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+benzyl=C8H9#+toluene     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11     0.0        13.1E3             !
<estimated(t")>!
etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11    0.0        13.1E3          !
<estimated(t")>!
etC6H5+C5H5#=C8H9#+C5H6#        1.1E11     0.0        13.1E3          !
<estimated(t")>!

!t": estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2      7.2E8      1.5        6.79E3     !MF
correlation Dean-Bozzelli 2000
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```
etC6H5+B1O=C8H9#-1+R2OH          5.1E8      1.5        5.05E3          !MF
correlation Dean-Bozzelli 2000
etC6H5+R2OH=C8H9#-1+H2O          3.6E6      2.0        4.82E2     !MF
correlation Dean-Bozzelli 2000
etC6H5+R3OOH=C8H9#-1+H2O2  4.2E4      2.69  1.85E4          !MF
correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4   2.43E6     1.87  1.03E4     !MF correlation
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9#         5.27E13   0.0    12.0E3  !ajout MF as
2/3 toluene <HECKMANN96>!
etC6H5+C6H5#=C6H6#+C8H9#      5.27E13   0.0    9.0E3   !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1    5.85E10   0.0    3.83E3  !ajout MF as
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>


! Ajout ipso MF
etC6H5+B1O=C6H5O#+R11C2H5  1.7E13   0.0     3.6E3    !MF as toluene !
<TAPPE89>!
etC6H5+R2OH=C6H5OH#+R11C2H5  1.3E13   0.0    10.6E3    !MF as toluene
<BAULCH94>as benzene
!etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.59E4    !MF as benzene
<Robaugh,J. Phys. Chem.90(1986)4159 - 4163>
etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.24E4    ! MF as benzene-
kcal <Robaugh,J. Phys. Chem.90(1986)4159 - 4163>

!** Decompositions

C8H9#-1=C2H4Z+C6H5#     2.0E13   0.0      35.5E3 !MF correlation exgas
C8H9#  =R1H+styrene        3.1e13   0.0      50670      !<MULLER88>
C8H9#-1=R1H+styrene        4.0E13   0.0      33.58E3    !MF <Sirjean,
J.Phys.Chem.A 2008>

!** Reactions of derived radicals
C8H9#+O2=R3OOH+styrene                      6.90E11          0.0
15.2E3      !<est (exgas-sylvain)>!

!C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO                  3.27E12          0.0
0.0      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R3OOH=R2OH+R1H+C6H5COCH3                  7.80E10          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R3OOH=>R2OH+C6H5#+CH3CHO                  2.54E11          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R3OOH=C8H9#OOH                             3.60E12          0.0
0.0   !MF KINGAS
C8H9#OOH=R2OH+C8H9#O                             5.00E15
0.0    42500          !MF
C8H9#O=R4CH3+C6H5CHO                             2.69E13          0.0
12117      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
C8H9#O=C6H5#+CH3CHO                                   1.74E14
0.0      20458        !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem
81(2003)431-442>
```

```
C8H9#-1+O2=R3OOH+styrene                    2.60E11          0.0
2.5E3
C8H9#-1+R3OOH=R2OH+HCHO+benzyl              5.00E12          0.0
0.0      !<kingas>!

!*****************************************!
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!
!*****************************************!

styrene+O2=R3OOH+C6H5C2H2          2.0E13       0.0        57.9E3  !
<asbutadiene/2>!
!C4H6Z2+O2=iC4H5+R3OOH             4.0E13       0.0        57.9E3  !
<LEUNG95>!


!styrene+B1O=C6H5#+R13CH2CHO        3.0E08       1.45        0.9E3  !
<asbutadiene/2>! ! ENLEVE PAR BENOIT ET PAG
styrene+R2OH=benzyl+HCHO           1.4E12       0.0        -0.9E3  !<as
butadiene/2!
styrene+R2OH=C6H5CHO+R4CH3         1.4E12       0.0        -0.9E3  !MF
idem rйaction prйcйdente as C3H6Y <TSAnG91>

!C4H6Z2+B1O=C3H5Y+R1H+B2CO          6.0E08       1.45        0.9E3  !
<LEUNG95,BREZINSKY84>!
!C4H6Z2+R2OH=C3H5Y+HCHO            2.8E12       0.0        -0.9E3  !
<LINSTEDT96>!
!C4H6Z2+R2OH=CH3CHO+R10C2H3V       5.6E12       0.0        -0.9E3  !
<fromLINSTEDT96>!

styrene+R1H=C6H5C2H2+H2            3.3E5        2.53        9.2E3  !MF<as
butadiene/2>!
styrene+R2OH=C6H5C2H2+H2O          1.5E6        2.0         0.4E3  !<as
butadiene/2>!
styrene+R4CH3=C6H5C2H2+CH4        3.5E13       0.0        15.5E3  !<as
butadiene/2>


!C4H6Z2+R1H=iC4H5+H2                6.6E5        2.53        9.2E3  !
<WANG97>!
!C4H6Z2+R2OH=iC4H5+H2O              3.1E6        2.0         0.4E3  !
<WANG97>!
!C4H6Z2+R4CH3=iC4H5+CH4             7.0E13       0.0        15.5E3  !
<WU87-3kcal>!

C6H5C2H2+O2=C6H5CO+HCHO             4.5E16      -1.39        1.0E3  !
<asMebel C2H3+O2>! **


!*Addition Zhenyu*!
C6H5C2H2+R1H=C6H5#C2H+H2                  1.0E13       0.0
0.0  !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and
Tech. 120 (1996) 119-167.
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C6H5C2H2+R2OH=C6H5#C2H+H2O         1.0E13       0.0           0.0  !in
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120
(1996) 119-167.

! ajout d'un amorcage Roda
C6H5#C2H   => C6H5# + R9C2H     2.2e16          0.0        98.0e3  ! MF
as toluene



!*****************************************!
!*REACTIONS OF C5H5CCH AND DERIVED RADICALS *!
!*****************************************!

!*Addition Zhenyu*!
!C5H5CCH=C5H5#+R9C2H                        4.2E15     0.0   125.0E3    !
<KInGAS1500>! pC3H4=R9C2H+R4CH3
!C5H5CCH+R1H=C5H5#+C2H2                     2.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R1H=C3H3+C4H4                      6.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R2OH=C5H5#+CH2COZ                  4.3E11     0.0         -0.8E3
     !<BOODAGHIAnS87>!pC3H4+R2OH=CH2COZ+R4CH3
!C5H4CCH2=C5H5CCH                       2.5E12     0.0    59.0E3    !
<HIDAKA89>!aC3H4=pC3H4
!C5H4CCH2+R1H=C5H5CCH+R1H               8.5E12     0.0     2.0E3    !
<WAGnER72>!aC3H4+R1H(+M)=tC3H5(+M)
!C5H4CCH2+R2OH=C5H5#+CH2COZ             2.0E12     0.0      -0.2E3 !<LIU88>!
aC3H4+R2OH=CH2COZ+R4CH3

!*****************************************!
!*REACTIONS OF BIBENZYL AND DERIVED RADICALS*!
!*****************************************!

bibenzyl=C14H13#+R1H                   1.0E16      0.0    83.66E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
bibenzyl+O2=C14H13#+R3OOH               2.8E12      0.0     35.0E3   !<est
aaaa!
bibenzyl+R1H=C14H13#+H2                    5.4E4       2.5     -1.9E3   !
Table A-I-21 Zhenyu

bibenzyl+B1O=C14H13#+R2OH               8.4E11      0.0       -2.0   !
<estimated(t"')>!
bibenzyl+R2OH=C14H13#+H2O               7.0E9           1.0    -1.13E3   !
<estimated(t"')>!

bibenzyl+R3OOH=C14H13#+H2O2             5.4E11      0.0   12.0E3   !
<estimated(t"')>!
bibenzyl+R4CH3=C14H13#+CH4              2.2E12      0.0      9.1E3   !
<estimated(t"')>!
bibenzyl+C6H5O#=C14H13#+C6H5OH#           2.2E12      0.0     13.1e3   !
<estimated(t"')>!
bibenzyl+benzyl=C14H13#+toluene         2.2E12      0.0    9.1E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
```

```
bibenzyl+C3H5Y=C14H13#+C3H6Y          2.2E12      0.0   13.1E3   !
<estimated(t"')>!
!t"': estimated as toluene with A x(4/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF
bibenzyl+R1H=C6H6#+C8H9#-1        5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet as toluene
bibenzyl+R2OH=C6H5OH#+C8H9#-1      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006
C14H13#=stilbene+R1H               7.94E15  0.0   51.864E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
C14H13#+O2= stilbene+R3OOH         1.6E12  0.00  15200  !as allylique
C14H13#+R3OOH=>R2OH+C6H5CHO+benzyl  8.21E4   2.20  -5.13E3 ! as benzyl

!*********************************************!
!*REACTIONS OF STILBENE                       *!
!*********************************************!
!Ajout Ipso MF
stilbene+R1H=>C6H6#+C2H2+C6H5#      5.67E8   1.43   5.65E3  !Calcul CBS-
QB3 Fournet as toluene
stilbene+R2OH=C6H5OH#+C6H5C2H2      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006

! ajout MF
stilbene+R2OH=C6H5CHO+benzyl       1.0E13       0.0        5.94E3  !
<Baulch05> as C2H4

!*****************************************************!
!* Reactions of naphthalene                          *!
!*****************************************************!
2C5H5#=naphthalene+H2           4.3E36  -6.3  22.835E3 ! A.M. Dean, J.
Phys. Chem. 94 (1990) 1432-1439.
C6H5#+iC4H3=naphthalene         3.18E23 -3.2  2.13E3   ! H.Y. Zhang, J.T.
McKinnon, CST 107 (1995) 261-300.
C6H5#+C4H4=naphthalene+R1H      3.3E33  -5.7  12.75E3  ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
benzyl+C3H3=>naphthalene+R1H+R1H 6.0E11  0.0  0.0      ! M.B. Colket,
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
C6H5C2H2+C2H2=naphthalene+R1H   1.6E16  -1.33 3.3E3    ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.


naphthalene+O2=R3OOH+naphthyl          8.0E13      0.0        63.4E3   !
like benzene <ALZUETA00>A*8/6!
naphthalene+B1O=>indenyl+B2CO+R1H      2.7E13      0.0      3.6E3   !like
benzene <Nicovich82>A*8/6!
naphthalene+R1H=naphthyl+H2            8.0E8       1.8     16.8E3  !like
benzene <MEBEL97>A*8/6!
naphthalene+B1O=naphthyl+R2OH          2.7E13      0.0     14.7E3  !like
benzene <LINDSTEDT94>A*8/6!
```

```
naphthalene+R2OH=naphthyl+H2O          2.1E8       1.42    1.45E3  !like
benzene <BAULCH92>A*8/6!
naphthalene+R3OOH=naphthyl+H2O2        7.3E12      0.0     28.9E3  !like
benzene <BAULCH94>A*8/6!
naphthalene+R4CH3=naphthyl+CH4         2.7E12      0.0     15.0E3  !like
benzene <ZHANG89>A*8/6!

naphthyl+R1H=naphthalene          1.0E14   0.0   0.0E3  !as n-
buthylbenzene
naphthyl+O2=>indenyl+B2CO+B1O     2.6E13   0.0   6.1E3  !as n-
buthylbenzene
naphthyl+B1O=>indenyl+B2CO        1.0E14   0.0   0.0    !as n-
buthylbenzene
naphthyl+R3OOH=>indenyl+B2CO+R2OH 5.0E12   0.0   0.0    !as n-
buthylbenzene
naphthyl+R2OH=>indenyl+B2CO+R1H   1.0E13   0.0   0.0    !as n-
buthylbenzene

!************************************************!
!* Reactions of indene and derived radicals       *!
!  Indene C6H4#/CH2/CH//CH/                      *!
!  Indenyl C6H4#/CH/CH//CH/                      *!
!  ph#C3H2  C6H5#/CH(.)/C///CH                   *!
!************************************************!

indene+R2OH=>C2H4Z+C6H5CO             1.37E12  0.0  -1.04E3  !Slavinskaya
indene+R2OH=>R10C2H3V+B2CO+C6H6#      1.37E12  0.0  -1.04E3 !Est.
!indene+R2OH=>o-methylbenzyl+B2CO     1.37E12  0.0  -1.04E3

indene+O2=R3OOH+indenyl               1.4E12   0.0   31.03E3  ! as n-
buthylbenzene mais E = DH de reaction
indene+B1O=indenyl+R2OH               1.76E11  0.7   3.25E3  ! A-I-21
secondary  A*2
indene+R1H=indenyl+H2                 1.08E5   2.5   -1.9E3  ! A-I-21
secondary  A*2
indene+R2OH=indenyl+H2O               6.0E6    2.0   -1.52E3 ! A-I-21
secondary  A*2
indene+R4CH3=indenyl+CH4              2.0E11   0.0   7.3E3   ! A-I-21
secondary  A*2
indene+R3OOH=H2O2+indenyl             1.28E4   2.6   12.4E3  ! A-I-21
secondary  A*2

!indene+R1H=ph#C3H4Y         5.8E13  0.0  8.1E3  !ipso-addition
!indene+R1H=ph#C3H4-1        5.8E13  0.0  8.1E3  !ipso-addition
indene+R1H=>C2H2+benzyl       1.16E14  0.0  8.1E3 !mf 2x ipso-addition

indenyl=>C5H5#+C4H2           5.0E13   0.0  75.0E3  !Slavinskaya09
5.0E13  0.0  37.5E3
indenyl+R1H=indene           1.0E14   0.0   0.0    !as n-buthylbenzene
C6H5#+C3H3=indene            6.46E12  0.0   0.0    !Slavinskaya09
!indenyl+R3OOH=>C6H6#+B2CO+R9C2H+R2OH    3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2
indenyl+R3OOH=>C6H5#C2H+R5CHO+R2OH         3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2
```

```
indenyl+B1O=>C6H6#+B2CO+R9C2H          5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H
indenyl+B1O=>C6H5#C2H+R5CHO           5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H

indenyl+R2OH=>styrene+B2CO   4.0E14   0.0   4.5E3  !Est.
C5H5#+OH=C4H6Z2+CO

!C9H7O#=C9H6O#+R1H          2.0E13  0.0  27.5E3   ! Est.like ph#CH2O
!C9H7O#=>C6H6#+B2CO+R9C2H   2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO
!C9H7O#=C6H5#C2H+R5CHO      2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO


!END
END
```

The mechanism for the oxidation of fuel blend methyl hexanoat/ n-heptane/toluene.

```
ELEMENTS
H O C N AR
END
SPECIES

! Biradicals :
B1O
B2CO
B3C
B4CH
B5CH2
B6CH2

! Primary molecules :
! Reactants:
C7H16-1
C8H18-1
H2
```

H2O
O2
H2O2
CH4
HCHO
CH3OH
CO2
CH3OOH
C2H2
C2H4Z
C2H6
CH2COZ
CH3CHO
C2H5OH
C2H3OH
C2H5OOH
CH3COOOH
C3H6Y
C3H8
C4H8Y
C4H10
C2H5CHO
C3H7OH
C2H6CO
C3H8CO
C4H6Z2
C2H3CHOZ
C7H16
C8H18
C5H10Z
C7H14Z
C6H12Z
C7H14Y
C8H16Y
C8H16Z
C5H10Y
C4H10OL
C4H10O2P
C3H8O2P
C5H12
C5H10OA
C4H8OA
C5H12OL
C6H14

! Secondary molecules :
C6H12OA
C7H14OA
C9H18Z
C10H20Z
C13H26Z
C12H24Z
C11H22Z
!C14H28Z

C8H16OA
C9H18OA
C12H24OA
C11H22OA
C10H20OA
C13H26OA
C3H6OLY
C3H6O2PY
C4H6OAY
C4H8OLY
C6H10Y2
C7H12Y2
C10H18Y2
C11H20Y2
C8H14Y2
C4H8O2PY
C5H8OAY
C5H10OLY
C12H22Y2
C9H16Y2
C7H14OLY
C7H14O2PY
C8H14OAY
C8H16OLY
!C14H26Y2
!C15H28Y2
C8H16O2PY
C9H16OAY
C9H18OLY
!C16H30Y2
C13H24Y2
C5H10O2PY
C6H10OAY
C6H12OLY
C4H6OKZ
C5H8OKZ
C6H10OKZ
C7H12OKZ

! Cyclic primary molecules :
C2H4OE#3

! Cyclic secondary molecules :
C3H6OE#3
C4H8OE#3
C5H10OE#3
C7H14OE#3
C6H12OE#3
C8H16OE#3
C9H18OE#3
C10H20OE#3
C13H26OE#3
C12H24OE#3
C11H22OE#3

```
!C14H28OE#3

! Benzenic primary molecules :

! Free radicals :
R1H   !   .h
R2OH   !   .oh
R3OOH   !   .o/oh
R4CH3   !   .ch3
R5CHO   !   .ch//o
R6CH2OH   !   .ch2/oh
R7CH3O   !   .o/ch3
R8CH3OO   !   .o/o/ch3
R9C2H   !   .c///ch
R10C2H3V   !   .ch//ch2
R11C2H5   !   .ch2/ch3
R12CHCOZ   !   .ch//c//o
R13CH2CHO   !   .ch2/ch//o
R14CH3CO   !   .c(//o)/ch3
R15C2H5O   !   .o/ch2/ch3
R16C2H4OOH   !   .ch2/ch2/o/oh
R17C2H5OO   !   .o/o/ch2/ch3
R18CH3COOO   !   .o/o/c(//o)/ch3
R19C3H7   !   .ch2/ch2/ch3
R20C4H9   !   .ch2/ch2/ch2/ch3
R21CH3OCO   !   .c(//o)/o/ch3
!R22CO2H   !   .c(//o)/oh
!R23C2H3O2B   !   .ch2/c(//o)/oh
!R24C2H4OH   !   .ch2/ch2/oh
!R25C2H4OH   !   .ch(/oh)/ch3
R23C2H4OH   !   c.h2-ch2-oh
R24C2H4OH   !   ch3-c.h-oh
R25C2H5CO   !   ch3-ch2-c.o

R26C7H15   !   .ch(/ch2/ch2/ch3)2
R27C7H15   !   .ch2/ch2/ch2/ch2/ch2/ch2/ch3
R28C7H15   !   .ch(/ch3)/ch2/ch2/ch2/ch2/ch3
R29C7H15   !   .ch(/ch2/ch3)/ch2/ch2/ch2/ch3
R30C8H17   !   .ch2/c(/ch3)2/ch2/ch(/ch3)2
R31C8H17   !   .ch2/ch(/ch3)/ch2/c(/ch3)3
R32C8H17   !   .c(/ch3)2/ch2/c(/ch3)3
R33C8H17   !   .ch(/ch(/ch3)2)/c(/ch3)3
R34C4H9   !   .ch(/ch3)/ch2/ch3
R35C5H11   !   .ch2/ch2/ch2/ch2/ch3
R36C4H9   !   .ch2/ch(/ch3)2
R37C5H11   !   .ch2/c(/ch3)3
R38C4H9   !   .c(/ch3)3
R39C5H11   !   .ch(/ch2/ch3)2
R40C5H11   !   .ch(/ch3)/ch2/ch2/ch3
R41C6H13   !   .ch2/ch2/ch2/ch2/ch2/ch3
R42C7H15   !   .c(/ch3)2/ch2/ch(/ch3)2
R43C3H7   !   .ch(/ch3)2
R44C7H15   !   .ch(/ch3)/ch2/c(/ch3)3
 !Cyclic free radicals:
```

```
 !Benzenic free radicals:

! lumped Free radicals :
RC3H5Y
RC4H7Y
RC3H5O
RC7H13Y
RC8H15Y
RC5H9Y
RC5H9O
RC4H7O
RC3H5O3
RC6H11O
RC7H13O
RC5H9O3
RC4H7O3
RC6H11O3
RC7H13O3
RC8H15O
RC9H17O
RC12H23O
RC11H21O
RC10H19O
RC13H25O
RC8H15O3
RC9H17O3
RC11H23
RC12H23O3
RC10H21
RC11H21O3
RC9H19
RC10H19O3
RC12H25
RC13H25O3
RC6H11Y
! lumped Cyclic free radicals :

N2
AR

!!!!!!!!!!Espиces rajoutйes pour le mйca toluиne

aC3H4      !ch2//ch//ch2                        propadiene = allene
pC3H4      !ch///c/ch3                               propyne
C4H2       !ch///c/c///ch                       butadiyne = diacetylene
C4H4       !ch2//ch/c///ch                      1-buten-3-yne ou vinyl
acetylene
C4H6-12          !ch2//c//ch/ch3                     1,2-butadiиne ou
mйthyl allиne
C4H6-1           !ch///c/ch2/ch3                     1-butyne
C4H6-2           !ch3/c///c/ch3                      2-butyne
iC4H8      !ch2//c(ch3)/ch3               2methyl-propene
C5H8       !ex ch2//ch/ch2/ch//ch2        pentadiene
iC5H8      !ex ch3/c(ch3)//c//ch2
```

```
!iC5H10         !ex ch3/ch(ch3)/ch//ch2
!C5H10          !ex ch2//ch/ch2/ch2/ch3         pentene
C5H8#       !c(#1)h2/ch2/ch//ch/ch2/1       cyclopentene
C5H6#       !c(#1)h//ch/ch//ch/ch2/1        cyclopentadiene
C6H6#       !c(#1)h&ch&ch&ch&ch&ch&1        benzene
toluene         !c(#1)h&ch&ch&ch&ch&ch&1(/ch3)
MCP             !c(#1)h2/ch2/ch//ch/ch(/ch3)/1  methylcyclopentene
MCPD        !c(#1)h//ch/ch//ch/ch(/ch3)/1   methylcyclopentadiene
C5H4O#          !o//c(#1)/ch//ch/ch//ch/1
C3H2        !.ch//c//c(.)h
C2H4O#3     !c(#1)h2/o/ch2/1
C2H3CHO         !ch(//o)/ch//ch2                2-propenal
cC3H4       !c(#1)h2/ch//ch/1                   cyclopropene
cC3H6       !c(#1)h2/ch2/ch2/1                  cyclopropane
tC4H4       !ch2//c//c//ch2                     1,2,3 butatriene
C6H2        !ch///c/c///c/c///ch            hexatriyne
cC4H6       !c(#1)h2/ch//ch/ch2/1               cyclobutene
lC6H4       !ch///c/ch//ch/c///ch
!lC6H6          !ch2//ch/c///c/ch//ch2      !MF car n'intervient plus (une
rйaction)
lC6H8       !ch2//ch/ch//ch/ch//ch2
C6H8#       !c(#1)h2/ch//ch/ch2/ch//ch/1    cyclohexadiene
C6H10#          !c(#1)h2/ch//ch/ch2/ch2/ch2/1   cyclohexene
C8H10#          !c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1   cyclooctatriene
!Especes excitees
OHE
CHE
iC3H7       !.ch(/ch3)2
C3H3        !ch///c/ch2(.)
C3H5Y       !.ch2/ch//ch2
tC3H5       !ch2//c(.)/ch3
sC3H5       !.ch//ch/ch3
nC4H3       !.ch//ch/c///ch
iC4H3       !ch2//c(.)/c///ch
nC4H5       !.ch//ch/ch//ch2
iC4H5       !ch2//c(.)/ch//ch2
C4H5-1s         !ch///c/ch(.)/ch3
C4H5-1p         !.ch2/ch2/c///ch
C4H5-2          !.ch2/c///c/ch3
lC6H5       !ch///c/ch//ch/ch//ch(.)
lC6H7       !ex .ch//ch/ch//ch/ch//ch2
!lC6H9          !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus (une
rйaction)
C6H4#       !.c(#1)&ch&ch&ch&ch&c(.)&1
C6H5#       !.c(#1)&ch&ch&ch&ch&ch&1
C6H7#       !.c(#1)h/ch//ch/ch2/ch//ch/1
C6H9Z#          !.c(#1)h/ch//ch/ch2/ch2/ch2/1
C4H7-1          !.ch2/ch2/ch//ch2
C4H7-2          !ch3/c(.)//ch/ch3
C4H7Y       !ch3/c(.)h/ch//ch2
C4H7T       !ch2//c(.)/ch2/ch3
iC4H7       !.ch//c(/ch3)2
C4H7V       !.c(/ch3)//ch/ch3
!C5H7Y          !ch2//ch/ch//ch/c(.)h2
```

```
!iC5H7Y          !ch2//c(/c(.)h2)/ch//ch2
C5H9Y      !ch2//ch/c(.)h/ch2/ch3
iC5H9      !.ch2/ch(/ch3)/ch//ch2
!iC5H9Y          !ch3/c(.)(/ch3)/ch//ch2
CH2CHCO          !.ch2/ch//c//o
cC3H3      !.c(#1)h/ch//ch/1
! MECHANISM OF BENZENE
! Molecules
C4H4O      !ch2//ch/ch//c//o                              vinylketene
!lC5H6           !ch///c/ch//ch/ch3                              !MF car
n'intervient plus (une rйaction)
C5H5OH#          !c(#1)h//ch/ch//ch/ch(/oh)/1          cyclopentadienol
C6H5OH#          !c(#1)h&ch&ch&ch&ch&c(/oh)&1          phйnol
OC6H4O           !o//c(#1)/ch//ch/ch//ch/c(//o)/1      orthobenzoquinone
C6H5#C2H   !ch///c/c(#1)&ch&ch&ch&ch&ch/&1       phenylacetylene
etC6H5           !c(#1)h&ch&ch&ch&ch&c(/ch2/ch3)&1     ethylbenzene
styrene          !c(#1)h&ch&ch&ch&ch&c(/ch//ch2)&1
!C6H5C3H3  !c(#1)h&ch&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus
(une rйaction)
C10H10#          !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1 !
bicyclopentadienyl
C6H5CHO          !c(#1)h&ch&ch&ch&ch&c(/ch//o)&1       benzaldehyde
biphenyl   !c(#1)h&ch&ch&ch&ch&c(/c(#2)h&ch&ch&ch&ch&c&2)&1
C6H5OOH

! Radicals
C5H5#      !c(#1)(.)h/ch//ch/ch//ch/1
lC5H5      !.c///c/ch//ch/ch3
C5H3O#           !.c(#1)//ch/ch//ch/c(//o)&1
C5H5O#           !c(#1)h//ch/ch//ch/ch(/o(.))&1
C5H4OH#          !.c(#1)//ch/ch//ch/ch(/oh)&1
C6H5O#           !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5O2           !.c(#1)&ch&ch&ch&ch&c(/o/o(.))&1
C6H4OH#          !.c(#1)&ch&ch&ch&ch&c(/oh)&1
OC6H4OH          !c(#1)h&ch&ch&ch&ch(/o(.))&c(/oh)&1


!MECHANISM OF TOLUENE
HOC6H4CH3  !oh/c(#1)&ch&ch&ch&ch&c(/ch3)&1 cresol
C6H4OHCHO  !oh/c(#1)&ch&ch&ch&ch&c(/ch//o)&1
C6H5CH2OH  !c(#1)h&ch&ch&ch&ch&c(/ch2/oh)&1
C6H5CH2OOH !c(#1)h&ch&ch&ch&ch&c(/ch2/o/oh)&1
bibenzyl   !ok
stilbene   !ok
benzyl           !c(#1)h&ch&ch&ch&ch&c(/c(.)h2)&1
C6H4CH3          !c(#1)h&ch&ch&ch&ch&c(/ch3)&1
C6H4OHCO   !oh/c(#1)&ch&ch&ch&ch&c(/c(.)//o)&1
HOC6H4CH2OO !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o/o(.))&1
OC6H4CH3   !o(.)/c(#1)&ch&ch&ch&ch&c(/ch3)&1
HOC6H4CH2  !oh/c(#1)&ch&ch&ch&ch&c(/c(.)h2)&1
C6H5CO           !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5CHOH   !c(#1)h&ch&ch&ch&ch&c(/c(.)h/oh)&1
C6H5CH2O   !c(#1)h&ch&ch&ch&ch&c(/ch2/o(.))&1
HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o(.))&1
```

```
C6H5CH2OO  !c(#1)h&ch&ch&ch&ch&c(/ch2/o/o(.))&1
C8H9#      !c(#1)h&ch&ch&ch&ch&c(/c(.)h2/ch2)&1
C8H9#-1          !c(#1)h&ch&ch&ch&ch&c(/ch2/c(.)h2)&1
C6H5C2H2   !c(#1)h&ch&ch&ch&ch&c(/ch//c(.)h)&1
C14H13#          !bibenzyl -H



!MECHANISM OF CYCLOPENTENE!
!C5H8-12         !ch2//c//ch/ch2/ch3
!C5H7#           !.c(#1)h/ch2/ch//ch/ch2/1
!C5H7#Y          !c(#1)h2/c(.)h/ch//ch/ch2/1
!C5H7#V          !c(#1)h2/ch2/c(.)//ch/ch2/1
!C5H7-1s         !ch(.)//ch/ch2/ch//ch2
!C5H7-2t         !ch2//ch/ch2/c(.)//ch2
!C5H7-4t         !ch3/c(.)//ch/ch//ch2
!C5H7-3t         !ch3/ch//c(.)/ch//ch2
!C5H7-5p         !ch2(.)/ch2/ch2/c///ch
!C5H7-12-5p      !ch2(.)/ch2/ch//c//ch2
!C5H9#           !.c(#1)h/ch2/ch2/ch2/ch2/1
!C5H9      !(.)ch2/ch2/ch2/ch//ch2
!RMCP1           !c(#1)h(.)/ch2/ch//ch/ch(/ch3)/1
!RMCP2           !c(#1)h2/ch2/ch//ch/ch(/ch2(.))/1
!RMCPY1          !c(#1)h2/ch(.)/ch//ch/ch(/ch3)/1
!RMCPY2          !c(#1)h2/ch2/ch//ch/c(.)(/ch3)/1
!RMCPD           !c(#1)h//ch/ch//ch/ch(/ch2(.))/1
!RMCPDY          !c(#1)h//ch/ch//ch/c(.)(/ch3)/1

!*Especes ajoutйes*!
!mfC5H5C2H2      !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1
!C5H4CCH2  !c(#1)h//ch/ch//ch/c(//c//ch2)/1
!C5H5CCH   !c(#1)h//ch/ch//ch/ch(/c///ch)/1
!C6H5COCH3 !C6H5x/CO/CH3
C8H9#OOH   !C6H5#ch(/ooh)/ch3 ! c(#1)h&ch&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1
C8H9#O           !C6H5#ch(/o(.))/ch3 !
c(#1)h&ch&ch&ch&ch&c(/ch(/o(.))/ch3)&1
OOC6H4CH3  !o(.)/o/c(#1)&ch&ch&ch&ch&c(/ch3)&1
!C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!TolOCH2C6H5  !ch3/c(#1)&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolCH2bz     !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
CH3bzOHCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!Benzaldtol      !
c(#1)h&ch&ch&ch&ch&c(/c(//o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1
!HOC6H4CHO  !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1
!C6H5C4H7   !c(#1)h&ch&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1
naphthalene
!benzofuran
C8H8O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2
C8H7O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch(.)/ch2/2
C8H7O#-1        ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch(.)/2
naphthyl
indenyl
indene
```

```
!cumene
!CH3styre
C9H11#-1
C2H3C6H4CH2
!phenanthrene
!C6H5CH2CHO
!!!!!!!!!!!!!!!!!!!!!!!!!
********************************************************************************
!!! MEtHylEtHaNOatE sPECiEs !!!
MEMj
ME2j       ME2*O      ME2j*O
!!! MEtHylPrOPaNOatE sPECiEs !!!
MP2j       MP3j       MP2D3j     MP2D2j     MP2DMj     MPMj
!!! MEtHylButaNOatE sPECiEs !!!
MB2j       MB3j       MB4j       MBMj
MB3D2j    MB2DMj     MB3DMj     MB2D3j

!!! MEtHylPENtaNOatE sPECiEs !!!
MPE5j      MPE4j      MPE3j      MPE2j      MPEMj      MPE4D3j    MPE4D2j
MPE3D2j    MPE4D2D    MPE
!
ME  MP  MP2D  MB  MP2D  MB3D  MB2D   MB2D-z  MB3D2O  MPE4D   MPE3D  MPE2D
!
NC4H9CO
CH3CHCO
C2H5CHO
C2H3CO
CH2CCO
C3H7CO
sC3H5CO
aC3H5CO
C2H3CO2
!C4H7-3 C4H7-4

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!! Methyl Hexanoate Species
!!!!!!!!!!!!!!
MHX        MHX5d      MHX4d      MHX3d      MHX2d
MHX6j      MHX5j      MHX4j      MHX3j      MHX2j      MHXmj
MHX5d4j         MHX4d3j         MHX3d2j
HXAoj  C5H8CO
!!!!!!!!!!
HCCCO

END

REACTIONS
!(k = A T**b exp(-E/RT)) A units: mole-cm-sec-K, E units cal/mole

!     -----------------
!     PRIMARY REACTIONS
!     -----------------
!   molecular elimination :
!   unimolecular initiations :
```

```
C7H16-1=>R19C3H7+R20C4H9    2.0E+0017  0.000  85750.3  ! UI 1 KB
C7H16-1=>R11C2H5+R35C5H11    1.6E+0017  0.000  85815.5  ! UI 2 KB
C7H16-1=>R4CH3+R41C6H13    3.2E+0017  0.000  87654.8  ! UI 3 KB
C8H18-1=>R4CH3+R42C7H15    1.2E+0018  0.000  81845.9  ! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9    2.4E+0017  0.000  78804.1  ! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11    4.6E+0017  0.000  83562.0  ! UI 6 KB
C8H18-1=>R4CH3+R44C7H15    8.0E+0017  0.000  87665.1  ! UI 7 KB

!   bimolecular initiations :
C7H16-1+O2=>R3OOH+R26C7H15    1.4E+0013  0.000  50652.5  ! BI 8 CN
C7H16-1+O2=>R3OOH+R27C7H15    4.2E+0013  0.000  53033.1  ! BI 9 CN
C7H16-1+O2=>R3OOH+R28C7H15    2.8E+0013  0.000  50588.2  ! BI 10 CN
C7H16-1+O2=>R3OOH+R29C7H15    2.8E+0013  0.000  50652.5  ! BI 11 CN
C8H18-1+O2=>R3OOH+R30C8H17    6.3E+0013  0.000  53033.0  ! BI 12 CN
C8H18-1+O2=>R3OOH+R31C8H17    4.2E+0013  0.000  52333.1  ! BI 13 CN
C8H18-1+O2=>R3OOH+R32C8H17    7.0E+0012  0.000  47243.3  ! BI 14 CN
C8H18-1+O2=>R3OOH+R33C8H17    1.4E+0013  0.000  50652.7  ! BI 15 CN

!   additions :

!   additions with oxygen:

!   isomerisations :
R20C4H9=R34C4H9    3.3E+0009  1.000  37000.0  ! IS 16 KB
R26C7H15=R28C7H15    6.7E+0009  1.000  37000.0  ! IS 17 KB
R26C7H15=R27C7H15    1.7E+0009  1.000  19800.0  ! IS 18 KB
R27C7H15=R29C7H15    9.9E+0007  1.000  37000.0  ! IS 19 KB
R27C7H15=R28C7H15    1.7E+0007  1.000  17400.0  ! IS 20 KB
R28C7H15=R29C7H15    5.7E+0008  1.000  17300.0  ! IS 21 KB
R30C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 22 KB
R30C8H17=R32C8H17    2.9E+0008  1.000  15300.0  ! IS 23 KB
R30C8H17=R31C8H17    3.0E+0008  1.000  14500.0  ! IS 24 KB
R31C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 25 KB
R35C5H11=R39C5H11    3.3E+0009  1.000  37000.0  ! IS 26 KB
R35C5H11=R40C5H11    5.7E+0008  1.000  17300.0  ! IS 27 KB

!   Decomposition of OOQOOH into branching agents:

!   beta-scissions :
R19C3H7=>R4CH3+C2H4Z    2.0E+0013  0.000  31000.0  ! DE 28 CN
R19C3H7=>R1H+C3H6Y    3.0E+0013  0.000  38000.0  ! DE 29 CN
R20C4H9=>R11C2H5+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 30 CW
R20C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 31 CN
R26C7H15=>R11C2H5+C5H10Z    4.0E+0013  0.000  28700.0  ! DE 32 CW
R26C7H15=>R1H+C7H14Z    6.0E+0013  0.000  38000.0  ! DE 33 CN
R27C7H15=>R35C5H11+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 34 CW
R27C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 35 CN
R28C7H15=>R20C4H9+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 36 CW
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 37 CN
     DUPLICATE
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 38 CN
     DUPLICATE
R29C7H15=>R19C3H7+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 39 CW
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 40 CN
```

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     DUPLICATE
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 41 CN
     DUPLICATE
R29C7H15=>R4CH3+C6H12Z    2.0E+0013  0.000  31000.0  ! DE 42 CN
R30C8H17=>R36C4H9+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 43 CW
R30C8H17=>R4CH3+C7H14Y    4.0E+0013  0.000  31000.0  ! DE 44 CN
R31C8H17=>R37C5H11+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 45 CW
R31C8H17=>R4CH3+C7H14Z    2.0E+0013  0.000  31000.0  ! DE 46 CN
R31C8H17=>R1H+C8H16Y    1.5E+0013  0.000  37500.0  ! DE 47 CN
R32C8H17=>R38C4H9+C4H8Y    2.0E+0013  0.000  26700.0  ! DE 48
R32C8H17=>R1H+C8H16Y    6.0E+0013  0.000  39000.0  ! DE 49 CN
R32C8H17=>R1H+C8H16Z    3.0E+0013  0.000  38000.0  ! DE 50 CN
R33C8H17=>R4CH3+C7H14Z    4.0E+0013  0.000  31000.0  ! DE 51 CN
R33C8H17=>R4CH3+C7H14Y    6.0E+0013  0.000  31000.0  ! DE 52 CN
R33C8H17=>R1H+C8H16Z    3.0E+0013  0.000  37500.0  ! DE 53 CN
R34C4H9=>R4CH3+C3H6Y    2.0E+0013  0.000  31000.0  ! DE 54 CN
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 55 CN
     DUPLICATE
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  39000.0  ! DE 56 CN
     DUPLICATE
R35C5H11=>R19C3H7+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 57 CW
R35C5H11=>R1H+C5H10Z    3.0E+0013  0.000  38000.0  ! DE 58 CN
R36C4H9=>R4CH3+C3H6Y    4.0E+0013  0.000  31000.0  ! DE 59 CN
R36C4H9=>R1H+C4H8Y    3.0E+0013  0.000  37500.0  ! DE 60 CN
R37C5H11=>R4CH3+C4H8Y    6.0E+0013  0.000  31000.0  ! DE 61 CN
R38C4H9=>R1H+C4H8Y    9.0E+0013  0.000  39000.0  ! DE 62 CN
R39C5H11=>R4CH3+C4H8Y    4.0E+0013  0.000  31000.0  ! DE 63 CN
R39C5H11=>R1H+C5H10Y    6.0E+0013  0.000  38000.0  ! DE 64 CN
R40C5H11=>R11C2H5+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 65 CW
R40C5H11=>R1H+C5H10Z    3.0E+0013  0.000  39000.0  ! DE 66 CN
R40C5H11=>R1H+C5H10Y    3.0E+0013  0.000  38000.0  ! DE 67 CN
R41C6H13=>R20C4H9+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 68 CW
R41C6H13=>R1H+C6H12Z    3.0E+0013  0.000  38000.0  ! DE 69 CN
R42C7H15=>R43C3H7+C4H8Y    2.0E+0013  0.000  27700.0  ! DE 70
R42C7H15=>R1H+C7H14Y    3.0E+0013  0.000  38000.0  ! DE 71 CN
     DUPLICATE
R42C7H15=>R1H+C7H14Y    6.0E+0013  0.000  39000.0  ! DE 72 CN
     DUPLICATE
R43C3H7=>R1H+C3H6Y    6.0E+0013  0.000  39000.0  ! DE 73 CN
R44C7H15=>R38C4H9+C3H6Y    2.0E+0013  0.000  26700.0  ! DE 74
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 75 CN
     DUPLICATE
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 76 CN
     DUPLICATE
! decomposition of R(.)CO free radicals

!   decomposition to o-rings :

!   oxidations :
R26C7H15+O2=>C7H14Z+R3OOH    3.9E+0012  0.000  5000.0  ! OX 77 CN
R27C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 78 CN
R28C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 79 CN
     DUPLICATE
R28C7H15+O2=>C7H14Z+R3OOH    8.1E+0011  0.000  5000.0  ! OX 80 CN
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     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 81 CN
     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 82 CN
     DUPLICATE
R31C8H17+O2=>C8H16Y+R3OOH    6.4E+0011  0.000  5000.0  ! OX 83 CN
R32C8H17+O2=>C8H16Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 84 CN
R32C8H17+O2=>C8H16Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 85 CN
R33C8H17+O2=>C8H16Z+R3OOH    6.4E+0011  0.000  5000.0  ! OX 86 CN
R38C4H9+O2=>C4H8Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 87 CW
R43C3H7+O2=>C3H6Y+R3OOH    2.3E+0012  0.000  5000.0  ! OX 88 CW

!   oxidations of R(.)(OH) radicals:

!   metathesis :
B1O+C7H16-1=>R2OH+R26C7H15    2.6E+0013  0.000  5200.0  ! ME 89 CW
B1O+C7H16-1=>R2OH+R27C7H15    1.0E+0014  0.000  7850.0  ! ME 90 CW
B1O+C7H16-1=>R2OH+R28C7H15    5.2E+0013  0.000  5200.0  ! ME 91 CW
B1O+C7H16-1=>R2OH+R29C7H15    5.2E+0013  0.000  5200.0  ! ME 92 CW
B1O+C8H18-1=>R2OH+R30C8H17    1.5E+0014  0.000  7850.0  ! ME 93 CW
B1O+C8H18-1=>R2OH+R31C8H17    1.0E+0014  0.000  7850.0  ! ME 94 CW
B1O+C8H18-1=>R2OH+R32C8H17    1.0E+0013  0.000  3280.0  ! ME 95 CW
B1O+C8H18-1=>R2OH+R33C8H17    2.6E+0013  0.000  5200.0  ! ME 96 CW
C7H16-1+R1H=>H2+R26C7H15    9.0E+0006  2.000  5000.0  ! ME 97 CW
C7H16-1+R1H=>H2+R27C7H15    5.7E+0007  2.000  7700.0  ! ME 98 CW
C7H16-1+R1H=>H2+R28C7H15    1.8E+0007  2.000  5000.0  ! ME 99 CW
C7H16-1+R1H=>H2+R29C7H15    1.8E+0007  2.000  5000.0  ! ME 100 CW
C8H18-1+R1H=>H2+R30C8H17    8.6E+0007  2.000  7700.0  ! ME 101 CW
C8H18-1+R1H=>H2+R31C8H17    5.7E+0007  2.000  7700.0  ! ME 102 CW
C8H18-1+R1H=>H2+R32C8H17    4.2E+0006  2.000  2400.0  ! ME 103 CN
C8H18-1+R1H=>H2+R33C8H17    9.0E+0006  2.000  5000.0  ! ME 104 CW
C7H16-1+R2OH=>H2O+R26C7H15    2.6E+0006  2.000  -765.0  ! ME 105 CW
C7H16-1+R2OH=>H2O+R27C7H15    5.4E+0006  2.000  450.0  ! ME 106 CW
C7H16-1+R2OH=>H2O+R28C7H15    5.2E+0006  2.000  -765.0  ! ME 107 CW
C7H16-1+R2OH=>H2O+R29C7H15    5.2E+0006  2.000  -765.0  ! ME 108 CW
C8H18-1+R2OH=>H2O+R30C8H17    8.1E+0006  2.000  450.0  ! ME 109 CW
C8H18-1+R2OH=>H2O+R31C8H17    5.4E+0006  2.000  450.0  ! ME 110 CW
C8H18-1+R2OH=>H2O+R32C8H17    1.1E+0006  2.000  -1865.0  ! ME 111 CW
C8H18-1+R2OH=>H2O+R33C8H17    2.6E+0006  2.000  -765.0  ! ME 112 CW
C7H16-1+R3OOH=>H2O2+R26C7H15    4.0E+0011  0.000  15500.0  ! ME 113 CN
C7H16-1+R3OOH=>H2O2+R27C7H15    1.2E+0012  0.000  17000.0  ! ME 114 CN
C7H16-1+R3OOH=>H2O2+R28C7H15    8.0E+0011  0.000  15500.0  ! ME 115 CN
C7H16-1+R3OOH=>H2O2+R29C7H15    8.0E+0011  0.000  15500.0  ! ME 116 CN
C8H18-1+R3OOH=>H2O2+R30C8H17    1.8E+0012  0.000  17000.0  ! ME 117 CN
C8H18-1+R3OOH=>H2O2+R31C8H17    1.2E+0012  0.000  17000.0  ! ME 118 CN
C8H18-1+R3OOH=>H2O2+R32C8H17    2.0E+0011  0.000  14000.0  ! ME 119 CN
C8H18-1+R3OOH=>H2O2+R33C8H17    4.0E+0011  0.000  15500.0  ! ME 120 CN
C7H16-1+R4CH3=>CH4+R26C7H15    2.0E+0011  0.000  9600.0  ! ME 121 CN
C7H16-1+R4CH3=>CH4+R27C7H15    6.0E-0001  4.000  8200.0  ! ME 122 CN
C7H16-1+R4CH3=>CH4+R28C7H15    4.0E+0011  0.000  9600.0  ! ME 123 CN
C7H16-1+R4CH3=>CH4+R29C7H15    4.0E+0011  0.000  9600.0  ! ME 124 CN
C8H18-1+R4CH3=>CH4+R30C8H17    9.0E-0001  4.000  8200.0  ! ME 125 CN
C8H18-1+R4CH3=>CH4+R31C8H17    6.0E-0001  4.000  8200.0  ! ME 126 CN
C8H18-1+R4CH3=>CH4+R32C8H17    1.0E+0011  0.000  7900.0  ! ME 127 CW
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C8H18-1+R4CH3=>CH4+R33C8H17    2.0E+0011  0.000  9600.0  ! ME 128 CN
C7H16-1+R5CHO=>HCHO+R26C7H15    1.0E+0007  1.900  17000.0  ! ME 129 CN
C7H16-1+R5CHO=>HCHO+R27C7H15    2.0E+0005  2.500  18500.0  ! ME 130 CN
C7H16-1+R5CHO=>HCHO+R28C7H15    2.2E+0007  1.900  17000.0  ! ME 131 CN
C7H16-1+R5CHO=>HCHO+R29C7H15    2.2E+0007  1.900  17000.0  ! ME 132 CN
C8H18-1+R5CHO=>HCHO+R30C8H17    3.1E+0005  2.500  18500.0  ! ME 133 CN
C8H18-1+R5CHO=>HCHO+R31C8H17    2.0E+0005  2.500  18500.0  ! ME 134 CN
C8H18-1+R5CHO=>HCHO+R32C8H17    3.4E+0004  2.500  13500.0  ! ME 135 CN
C8H18-1+R5CHO=>HCHO+R33C8H17    1.0E+0007  1.900  17000.0  ! ME 136 CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15    6.0E+0001  2.950  12000.0  ! ME 137 CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15    2.0E+0002  2.950  14000.0  ! ME 138 CN
C7H16-1+R6CH2OH=>CH3OH+R28C7H15    1.2E+0002  2.950  12000.0  ! ME 139 CN
C7H16-1+R6CH2OH=>CH3OH+R29C7H15    1.2E+0002  2.950  12000.0  ! ME 140 CN
C8H18-1+R6CH2OH=>CH3OH+R30C8H17    3.0E+0002  2.950  14000.0  ! ME 141 CN
C8H18-1+R6CH2OH=>CH3OH+R31C8H17    2.0E+0002  2.950  14000.0  ! ME 142 CN
C8H18-1+R6CH2OH=>CH3OH+R32C8H17    1.2E+0002  2.760  10800.0  ! ME 143 CN
C8H18-1+R6CH2OH=>CH3OH+R33C8H17    6.0E+0001  2.950  12000.0  ! ME 144 CN
C7H16-1+R7CH3O=>CH3OH+R26C7H15    1.5E+0011  0.000  4500.0  ! ME 145 CN
C7H16-1+R7CH3O=>CH3OH+R27C7H15    3.2E+0011  0.000  7300.0  ! ME 146 CN
C7H16-1+R7CH3O=>CH3OH+R28C7H15    2.9E+0011  0.000  4500.0  ! ME 147 CN
C7H16-1+R7CH3O=>CH3OH+R29C7H15    2.9E+0011  0.000  4500.0  ! ME 148 CN
C8H18-1+R7CH3O=>CH3OH+R30C8H17    4.9E+0011  0.000  7300.0  ! ME 149 CN
C8H18-1+R7CH3O=>CH3OH+R31C8H17    3.2E+0011  0.000  7300.0  ! ME 150 CN
C8H18-1+R7CH3O=>CH3OH+R32C8H17    2.3E+0010  0.000  2900.0  ! ME 151 CN
C8H18-1+R7CH3O=>CH3OH+R33C8H17    1.5E+0011  0.000  4500.0  ! ME 152 CN
C7H16-1+R8CH3OO=>CH3OOH+R26C7H15    3.0E+0012  0.000  17500.0  ! ME 153
CN
C7H16-1+R8CH3OO=>CH3OOH+R27C7H15    1.2E+0013  0.000  20000.0  ! ME 154
CN
C7H16-1+R8CH3OO=>CH3OOH+R28C7H15    6.0E+0012  0.000  17500.0  ! ME 155
CN
C7H16-1+R8CH3OO=>CH3OOH+R29C7H15    6.0E+0012  0.000  17500.0  ! ME 156
CN
C8H18-1+R8CH3OO=>CH3OOH+R30C8H17    1.8E+0013  0.000  20000.0  ! ME 157
CN
C8H18-1+R8CH3OO=>CH3OOH+R31C8H17    1.2E+0013  0.000  20000.0  ! ME 158
CN
C8H18-1+R8CH3OO=>CH3OOH+R32C8H17    1.5E+0012  0.000  15000.0  ! ME 159
CN
C8H18-1+R8CH3OO=>CH3OOH+R33C8H17    3.0E+0012  0.000  17500.0  ! ME 160
CN
C7H16-1+R11C2H5=>C2H6+R26C7H15    2.0E+0011  0.000  11000.0  ! ME 161 CN
C7H16-1+R11C2H5=>C2H6+R27C7H15    6.0E+0011  0.000  13500.0  ! ME 162 CR
C7H16-1+R11C2H5=>C2H6+R28C7H15    4.0E+0011  0.000  11000.0  ! ME 163 CN
C7H16-1+R11C2H5=>C2H6+R29C7H15    4.0E+0011  0.000  11000.0  ! ME 164 CN
C8H18-1+R11C2H5=>C2H6+R30C8H17    9.0E+0011  0.000  13500.0  ! ME 165 CR
C8H18-1+R11C2H5=>C2H6+R31C8H17    6.0E+0011  0.000  13500.0  ! ME 166 CR
C8H18-1+R11C2H5=>C2H6+R32C8H17    1.0E+0011  0.000  9200.0  ! ME 167 CN
C8H18-1+R11C2H5=>C2H6+R33C8H17    2.0E+0011  0.000  11000.0  ! ME 168 CN
C7H16-1+R38C4H9=>C4H10+R26C7H15    1.0E+0011  0.000  12700.0  ! ME 169 CR
C7H16-1+R38C4H9=>C4H10+R27C7H15    3.0E+0011  0.000  15000.0  ! ME 170 CR
C7H16-1+R38C4H9=>C4H10+R28C7H15    2.0E+0011  0.000  12700.0  ! ME 171 CR
C7H16-1+R38C4H9=>C4H10+R29C7H15    2.0E+0011  0.000  12700.0  ! ME 172 CR
C8H18-1+R38C4H9=>C4H10+R30C8H17    4.5E+0011  0.000  15000.0  ! ME 173 CR
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C8H18-1+R38C4H9=>C4H10+R31C8H17    3.0E+0011  0.000  15000.0  ! ME 174 CR
C8H18-1+R38C4H9=>C4H10+R32C8H17    5.0E+0010  0.000  11100.0  ! ME 175 CR
C8H18-1+R38C4H9=>C4H10+R33C8H17    1.0E+0011  0.000  12700.0  ! ME 176 CR

!   combinations :
R1H+R38C4H9=>C4H10    8.3E+0012  0.000  0.0  ! CO 177 KB
R1H+R43C3H7=>C3H8    8.3E+0012  0.000  0.0  ! CO 178 KB
R2OH+R38C4H9=>C4H10OL    5.7E+0012  0.000  0.0  ! CO 179 KB
R2OH+R43C3H7=>C3H7OH    5.9E+0012  0.000  0.0  ! CO 180 KB
R3OOH+R38C4H9=>C4H10O2P    4.5E+0012  0.000  0.0  ! CO 181 KB
R3OOH+R43C3H7=>C3H8O2P    4.8E+0012  0.000  0.0  ! CO 182 KB
R4CH3+R38C4H9=>C5H12    1.5E+0013  0.000  0.0  ! CO 183 KB
R4CH3+R43C3H7=>C4H10    1.5E+0013  0.000  0.0  ! CO 184 KB
R5CHO+R38C4H9=>C5H10OA    4.9E+0012  0.000  0.0  ! CO 185 KB
R5CHO+R43C3H7=>C4H8OA    5.2E+0012  0.000  0.0  ! CO 186 KB
R6CH2OH+R38C4H9=>C5H12OL    4.8E+0012  0.000  0.0  ! CO 187 KB
R6CH2OH+R43C3H7=>C4H10OL    5.1E+0012  0.000  0.0  ! CO 188 KB
R11C2H5+R38C4H9=>C6H14    4.9E+0012  0.000  0.0  ! CO 189 KB
R11C2H5+R43C3H7=>C5H12    5.2E+0012  0.000  0.0  ! CO 190 KB
R38C4H9+R38C4H9=>C8H18    2.0E+0012  0.000  0.0  ! CO 191 KB
R38C4H9+R43C3H7=>C7H16    4.3E+0012  0.000  0.0  ! CO 192 KB
R43C3H7+R43C3H7=>C6H14    2.3E+0012  0.000  0.0  ! CO 193 KB

!   dismutations :

!    -------------------
!    SECONDARY MECHANISM
!    -------------------

!    Peroxide decomposition

! Hydroperoxide decomposition
C4H10O2P=>R2OH+R11C2H5+CH3CHO    1.5E+0016  0.000  43000.0  ! DHP 194
C3H8O2P=>R2OH+R11C2H5+HCHO    1.5E+0016  0.000  43000.0  ! DHP 195
C3H6O2PY=>R2OH+R1H+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 196
C4H8O2PY=>R2OH+R4CH3+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 197
C7H14O2PY=>R2OH+R20C4H9+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 198
C8H16O2PY=>R2OH+R35C5H11+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 199
C5H10O2PY=>R2OH+R11C2H5+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions
C3H8+R1H=>H2+R19C3H7    5.7E+0007  2.000  7700.0  ! MH 201
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     DUPLICATE
C3H8+R1H=>H2+R19C3H7    9.0E+0006  2.000  5000.0  ! MH 202
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    5.4E+0006  2.000  450.0  ! MH 203
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    2.6E+0006  2.000  -765.0  ! MH 204
     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    1.2E+0012  0.000  17000.0  ! MH 205
     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    4.0E+0011  0.000  15500.0  ! MH 206
     DUPLICATE
C3H8+R4CH3=>CH4+R19C3H7    6.0E-0001  4.000  8200.0  ! MH 207
     DUPLICATE
C3H8+R4CH3=>CH4+R19C3H7    2.0E+0011  0.000  9600.0  ! MH 208
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    1.2E+0013  0.000  20000.0  ! MH 209
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    3.0E+0012  0.000  17500.0  ! MH 210
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! MH 211
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    2.0E+0011  0.000  11000.0  ! MH 212
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    5.7E+0007  2.000  7700.0  ! MH 213
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    1.8E+0007  2.000  5000.0  ! MH 214
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.4E+0006  2.000  450.0  ! MH 215
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.2E+0006  2.000  -765.0  ! MH 216
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    1.2E+0012  0.000  17000.0  ! MH 217
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    8.0E+0011  0.000  15500.0  ! MH 218
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    6.0E-0001  4.000  8200.0  ! MH 219
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    4.0E+0011  0.000  9600.0  ! MH 220
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    1.2E+0013  0.000  20000.0  ! MH 221
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    6.0E+0012  0.000  17500.0  ! MH 222
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    6.0E+0011  0.000  13500.0  ! MH 223
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    4.0E+0011  0.000  11000.0  ! MH 224
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    5.7E+0007  2.000  7700.0  ! MH 225
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    2.7E+0007  2.000  5000.0  ! MH 226
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    5.4E+0006  2.000  450.0  ! MH 227
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    7.8E+0006  2.000  -765.0  ! MH 228
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     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  17000.0  ! MH 229
     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  15500.0  ! MH 230
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E-0001  4.000  8200.0  ! MH 231
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E+0011  0.000  9600.0  ! MH 232
     DUPLICATE
C5H12+R8CH3OO=>CH3OOH+R35C5H11    1.2E+0013  0.000  20000.0  ! MH 233
     DUPLICATE
C5H12+R8CH3OO=>CH3OOH+R35C5H11    9.0E+0012  0.000  17500.0  ! MH 234
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  13500.0  ! MH 235
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  11000.0  ! MH 236
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    5.7E+0007  2.000  7700.0  ! MH 237
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    3.6E+0007  2.000  5000.0  ! MH 238
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    5.4E+0006  2.000  450.0  ! MH 239
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    1.0E+0007  2.000  -765.0  ! MH 240
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.2E+0012  0.000  17000.0  ! MH 241
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.6E+0012  0.000  15500.0  ! MH 242
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    6.0E-0001  4.000  8200.0  ! MH 243
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    8.0E+0011  0.000  9600.0  ! MH 244
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  20000.0  ! MH 245
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  17500.0  ! MH 246
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    6.0E+0011  0.000  13500.0  ! MH 247
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    8.0E+0011  0.000  11000.0  ! MH 248
     DUPLICATE

! O-ring decomposition
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 249
     DUPLICATE
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    1.3E+0007  2.000  5000.0  ! DE# 250
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 251
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    3.9E+0006  2.000  -765.0  ! DE# 252
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  17000.0  ! DE# 253
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  15500.0  ! DE# 254
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     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 255
     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E+0011  0.000  9600.0  ! DE# 256
     DUPLICATE
C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    6.0E+0012  0.000  20000.0  ! DE#
257
     DUPLICATE
C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    4.5E+0012  0.000  17500.0  ! DE#
258
     DUPLICATE
C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
259
     DUPLICATE
C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  11000.0  ! DE#
260
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 261
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.3E+0007  2.000  5000.0  ! DE# 262
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 263
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    6.5E+0006  2.000  -765.0  ! DE# 264
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
265
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    1.0E+0012  0.000  15500.0  ! DE#
266
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 267
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    5.0E+0011  0.000  9600.0  ! DE# 268
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 269
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    7.5E+0012  0.000  17500.0  !
DE# 270
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
271
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    5.0E+0011  0.000  11000.0  ! DE#
272
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 273
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    3.2E+0007  2.000  5000.0  ! DE# 274
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 275
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    9.1E+0006  2.000  -765.0  ! DE# 276
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     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
277
     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    1.4E+0012  0.000  15500.0  ! DE#
278
     DUPLICATE
C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    3.0E-0001  4.000  8200.0  ! DE#
279
     DUPLICATE
C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    7.0E+0011  0.000  9600.0  ! DE#
280
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 281
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    1.0E+0013  0.000  17500.0  !
DE# 282
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    3.0E+0011  0.000  13500.0  !
DE# 283
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    7.0E+0011  0.000  11000.0  !
DE# 284
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 285
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    5.0E+0007  2.000  5000.0  ! DE# 286
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
287
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    1.4E+0007  2.000  -765.0  ! DE#
288
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 289
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    2.2E+0012  0.000  15500.0  !
DE# 290
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
291
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  9600.0  ! DE#
292
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 293
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    1.7E+0013  0.000
17500.0  ! DE# 294
     DUPLICATE
```

```
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 295
     DUPLICATE
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  11000.0  !
DE# 296
     DUPLICATE
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 297
     DUPLICATE
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    4.1E+0007  2.000  5000.0  ! DE# 298
     DUPLICATE
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
299
     DUPLICATE
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    1.1E+0007  2.000  -765.0  ! DE#
300
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 301
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    1.8E+0012  0.000  15500.0  !
DE# 302
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
303
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  9600.0  ! DE#
304
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 305
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    1.3E+0013  0.000
17500.0  ! DE# 306
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 307
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  11000.0  !
DE# 308
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE# 309
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    5.9E+0007  2.000  5000.0  ! DE# 310
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE# 311
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    1.7E+0007  2.000  -765.0  ! DE#
312
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    6.0E+0011  0.000  17000.0  ! DE#
313
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    2.6E+0012  0.000  15500.0  ! DE#
314
```

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     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
315
     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    1.3E+0012  0.000  9600.0  ! DE#
316
     DUPLICATE
C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    6.0E+0012  0.000  20000.0  !
DE# 317
     DUPLICATE
C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    2.0E+0013  0.000  17500.0  !
DE# 318
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 319
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    1.3E+0012  0.000  11000.0  !
DE# 320
     DUPLICATE
C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE# 321
     DUPLICATE
C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    6.8E+0007  2.000  5000.0  ! DE# 322
     DUPLICATE
C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE#
323
     DUPLICATE
C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.0E+0007  2.000  -765.0  ! DE#
324
     DUPLICATE
C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    6.0E+0011  0.000  17000.0  !
DE# 325
     DUPLICATE
C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    3.0E+0012  0.000  15500.0  !
DE# 326
     DUPLICATE
C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
327
     DUPLICATE
C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    1.5E+0012  0.000  9600.0  ! DE#
328
     DUPLICATE
C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    6.0E+0012  0.000
20000.0  ! DE# 329
     DUPLICATE
C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    2.3E+0013  0.000
17500.0  ! DE# 330
     DUPLICATE
C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 331
     DUPLICATE
C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    1.5E+0012  0.000  11000.0  !
DE# 332
     DUPLICATE
```

```
C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
333
     DUPLICATE
C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    7.7E+0007  2.000  5000.0  ! DE#
334
     DUPLICATE
C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
335
     DUPLICATE
C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.2E+0007  2.000  -765.0  ! DE#
336
     DUPLICATE
C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 337
     DUPLICATE
C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    3.4E+0012  0.000  15500.0  !
DE# 338
     DUPLICATE
C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    3.0E-0001  4.000  8200.0  ! DE#
339
     DUPLICATE
C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    1.7E+0012  0.000  9600.0  ! DE#
340
     DUPLICATE
C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 341
     DUPLICATE
C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    2.6E+0013  0.000  17500.0
! DE# 342
     DUPLICATE
C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    3.0E+0011  0.000  13500.0  !
DE# 343
     DUPLICATE
C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    1.7E+0012  0.000  11000.0  !
DE# 344
     DUPLICATE
C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
345
     DUPLICATE
C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    1.0E+0008  2.000  5000.0  ! DE#
346
     DUPLICATE
C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
347
     DUPLICATE
C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    3.0E+0007  2.000  -765.0  ! DE#
348
     DUPLICATE
C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 349
     DUPLICATE
C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    4.6E+0012  0.000  15500.0  !
DE# 350
     DUPLICATE
```

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C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 351
     DUPLICATE
C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    2.3E+0012  0.000  9600.0  !
DE# 352
     DUPLICATE
C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    6.0E+0012  0.000  20000.0
! DE# 353
     DUPLICATE
C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    3.5E+0013  0.000  17500.0
! DE# 354
     DUPLICATE
C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    3.0E+0011  0.000
13500.0  ! DE# 355
     DUPLICATE
C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    2.3E+0012  0.000
11000.0  ! DE# 356
     DUPLICATE
C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
357
     DUPLICATE
C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    9.5E+0007  2.000  5000.0  ! DE#
358
     DUPLICATE
C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
359
     DUPLICATE
C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0007  2.000  -765.0  ! DE#
360
     DUPLICATE
C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 361
     DUPLICATE
C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    4.2E+0012  0.000  15500.0  !
DE# 362
     DUPLICATE
C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 363
     DUPLICATE
C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    2.1E+0012  0.000  9600.0  !
DE# 364
     DUPLICATE
C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    6.0E+0012  0.000  20000.0
! DE# 365
     DUPLICATE
C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    3.2E+0013  0.000  17500.0
! DE# 366
     DUPLICATE
C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    3.0E+0011  0.000
13500.0  ! DE# 367
     DUPLICATE
C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    2.1E+0012  0.000
11000.0  ! DE# 368
     DUPLICATE
```

```
C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
369
     DUPLICATE
C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    8.6E+0007  2.000  5000.0  ! DE#
370
     DUPLICATE
C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
371
     DUPLICATE
C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.5E+0007  2.000  -765.0  ! DE#
372
     DUPLICATE
C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 373
     DUPLICATE
C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    3.8E+0012  0.000  15500.0  !
DE# 374
     DUPLICATE
C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    3.0E-0001  4.000  8200.0  ! DE#
375
     DUPLICATE
C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    1.9E+0012  0.000  9600.0  ! DE#
376
     DUPLICATE
C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 377
     DUPLICATE
C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    2.9E+0013  0.000  17500.0
! DE# 378
     DUPLICATE
C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    3.0E+0011  0.000  13500.0  !
DE# 379
     DUPLICATE
C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    1.9E+0012  0.000  11000.0  !
DE# 380
     DUPLICATE
!C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    2.9E+0007  2.000  7700.0  ! DE#
381
     DUPLICATE
!C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    1.1E+0008  2.000  5000.0  ! DE#
382
     DUPLICATE
!C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    2.7E+0006  2.000  450.0  ! DE#
383
     DUPLICATE
!C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    3.3E+0007  2.000  -765.0  !
DE# 384
     DUPLICATE
!C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    6.0E+0011  0.000  17000.0  !
DE# 385
     DUPLICATE
!C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    5.0E+0012  0.000  15500.0  !
DE# 386
     DUPLICATE
```

```
!C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    3.0E-0001  4.000  8200.0  !
DE# 387
     DUPLICATE
!C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    2.5E+0012  0.000  9600.0  !
DE# 388
     DUPLICATE
!C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    6.0E+0012  0.000
20000.0  ! DE# 389
     DUPLICATE
!C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    3.8E+0013  0.000
17500.0  ! DE# 390
     DUPLICATE
!C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    3.0E+0011  0.000  13500.0
! DE# 391
     DUPLICATE
!C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    2.5E+0012  0.000  11000.0
! DE# 392
     DUPLICATE


! Metatheses of oxetanes, furanes and pyranes

! decompositions of cyclo-ether radicals

! Addition of oxygen on cyclo-ether radicals
!    O2 elimination
!    Isomerization
!    Cylo-ether keto-hydroperoxide ester formation
!    Decomposition of cylo-ether keto-hydroperoxide ester

! Isomerization of peroxy-radicals

!Addition of oxygen on cyclo-peroxy radicals

! Formation of cyclo-ether ketohydroperoxydes

! Decomposition of cyclo-ether ketohydroperoxydes

! Olefin reactions
!  addition of H and CH3 on olefins
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  1560.0  ! ADZ 393
     DUPLICATE
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  3260.0  ! ADZ 394
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  1560.0  ! ADZ 395
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  3260.0  ! ADZ 396
     DUPLICATE
C4H8Y+R4CH3=>C3H6Y+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 397
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 398
     DUPLICATE
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 399
     DUPLICATE
C5H10Z+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 400
```

```
C5H10Z+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 401
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 402
     DUPLICATE
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 403
     DUPLICATE
C7H14Z+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 404
C7H14Z+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 405
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  1560.0  ! ADZ 406
     DUPLICATE
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  3260.0  ! ADZ 407
     DUPLICATE
C6H12Z+R4CH3=>C4H8Y+R19C3H7    1.7E+0011  0.000  7400.0  ! ADZ 408
C6H12Z+R4CH3=>C3H6Y+R20C4H9    9.6E+0010  0.000  8000.0  ! ADZ 409
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 410
     DUPLICATE
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 411
     DUPLICATE
C7H14Y+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 412
C7H14Y+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 413
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 414
     DUPLICATE
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 415
     DUPLICATE
C8H16Y+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 416
C8H16Y+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 417
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 418
     DUPLICATE
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 419
     DUPLICATE
C8H16Z+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 420
C8H16Z+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 421
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 422
     DUPLICATE
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 423
     DUPLICATE
C5H10Y+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 424
C5H10Y+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 425
C9H18Z+R4CH3=>C4H8Y+R41C6H13    1.7E+0011  0.000  7400.0  ! ADZ 426
C9H18Z+R4CH3=>C3H6Y+R26C7H15    9.6E+0010  0.000  8000.0  ! ADZ 427
C10H20Z+R4CH3=>C4H8Y+R26C7H15    1.7E+0011  0.000  7400.0  ! ADZ 428
C10H20Z+R4CH3=>C3H6Y+R30C8H17    9.6E+0010  0.000  8000.0  ! ADZ 429
C11H22Z+R4CH3=>C4H8Y+R30C8H17    1.7E+0011  0.000  7400.0  ! ADZ 430
C9H18Z+R1H=>4C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 431
C10H20Z+R1H=>4C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 432
C13H26Z+R1H=>6C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 433
C12H24Z+R1H=>5C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 434
C11H22Z+R1H=>5C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 435
!C14H28Z+R1H=>6C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 436

!  addition of OH on olefins
C3H6Y+R2OH=>R4CH3+CH3CHO    1.4E+0012  0.000  -1040.0  ! ADZ 437
C3H6Y+R2OH=>R11C2H5+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 438
C4H8Y+R2OH=>R4CH3+C2H5CHO    1.4E+0012  0.000  -1040.0  ! ADZ 439
C4H8Y+R2OH=>R19C3H7+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 440
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C5H10Z+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 441
C5H10Z+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 442
C7H14Z+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 443
C7H14Z+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 444
C6H12Z+R2OH=>R4CH3+C5H10OA    1.4E+0012  0.000  -1040.0  ! ADZ 445
C6H12Z+R2OH=>R35C5H11+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 446
C7H14Y+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 447
C7H14Y+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 448
C8H16Y+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 449
C8H16Y+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 450
C8H16Z+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 451
C8H16Z+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 452
C5H10Y+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 453
C5H10Y+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 454
C9H18Z+R2OH=>R4CH3+C8H16OA    1.4E+0012  0.000  -1040.0  ! ADZ 455
C9H18Z+R2OH=>R30C8H17+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 456
C10H20Z+R2OH=>R4CH3+C9H18OA    1.4E+0012  0.000  -1040.0  ! ADZ 457
C13H26Z+R2OH=>R4CH3+C12H24OA    1.4E+0012  0.000  -1040.0  ! ADZ 458
C12H24Z+R2OH=>R4CH3+C11H22OA    1.4E+0012  0.000  -1040.0  ! ADZ 459
C11H22Z+R2OH=>R4CH3+C10H20OA    1.4E+0012  0.000  -1040.0  ! ADZ 460
!C14H28Z+R2OH=>R4CH3+C13H26OA    1.4E+0012  0.000  -1040.0  ! ADZ 461

C10H20Z+R2OH=>HCHO+R4CH3+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 462
C13H26Z+R2OH=>HCHO+R11C2H5+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 463
C12H24Z+R2OH=>HCHO+R4CH3+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 464
C11H22Z+R2OH=>HCHO+R11C2H5+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 465
!C14H28Z+R2OH=>HCHO+R4CH3+6C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 466

!  addition of O on olefins
C3H6Y+B1O=>CH2COZ+R1H+R4CH3    1.2E+0005  2.560  -1130.0  ! AOZ 467
C4H8Y+B1O=>CH2COZ+R1H+R11C2H5    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Z+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Z+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C6H12Z+B1O=>CH2COZ+R1H+R20C4H9    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Y+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Y+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Z+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Y+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
C9H18Z+B1O=>CH2COZ+R1H+R26C7H15    1.2E+0005  2.560  -1130.0  ! AOZ 467
C10H20Z+B1O=>CH2COZ+R1H+R30C8H17    1.2E+0005  2.560  -1130.0  ! AOZ 467
!C13H26Z+B1O=>CH2COZ+R4CH3+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C12H24Z+B1O=>CH2COZ+R11C2H5+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467
!C11H22Z+B1O=>CH2COZ+R4CH3+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C14H28Z+B1O=>CH2COZ+R11C2H5+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467

! retroene reactions
C5H10Z=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 467
C7H14Z=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 468
C6H12Z=>C3H6Y+C3H6Y    8.0E+0012  0.000  56500.0  ! RTZ 469
C7H14Y=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 470
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C8H16Y=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 471
C8H16Z=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 472
C5H10Y=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 473
C9H18Z=>C3H6Y+C6H12Z    8.0E+0012  0.000  56500.0  ! RTZ 474
C10H20Z=>C3H6Y+C7H14Z    8.0E+0012  0.000  56500.0  ! RTZ 475
C13H26Z=>C3H6Y+C10H20Z    8.0E+0012  0.000  56500.0  ! RTZ 476
C12H24Z=>C3H6Y+C9H18Z    8.0E+0012  0.000  56500.0  ! RTZ 477
C11H22Z=>C3H6Y+C8H16Z    8.0E+0012  0.000  56500.0  ! RTZ 478
!C14H28Z=>C3H6Y+C11H22Z    8.0E+0012  0.000  56500.0  ! RTZ 479

!  addition of OOH on olefins
C3H6Y+R3OOH=>R2OH+C3H6OE#3    1.0E+0012  0.000  14200.0  ! ADZ 480
C4H8Y+R3OOH=>R2OH+C4H8OE#3    1.0E+0012  0.000  14200.0  ! ADZ 481
C5H10Z+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 482
C7H14Z+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 483
C6H12Z+R3OOH=>R2OH+C6H12OE#3    1.0E+0012  0.000  14200.0  ! ADZ 484
C7H14Y+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 485
C8H16Y+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 486
C8H16Z+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 487
C5H10Y+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 488
C9H18Z+R3OOH=>R2OH+C9H18OE#3    1.0E+0012  0.000  14200.0  ! ADZ 489
C10H20Z+R3OOH=>R2OH+C10H20OE#3    1.0E+0012  0.000  14200.0  ! ADZ 490
C13H26Z+R3OOH=>R2OH+C13H26OE#3    1.0E+0012  0.000  14200.0  ! ADZ 491
C12H24Z+R3OOH=>R2OH+C12H24OE#3    1.0E+0012  0.000  14200.0  ! ADZ 492
C11H22Z+R3OOH=>R2OH+C11H22OE#3    1.0E+0012  0.000  14200.0  ! ADZ 493
!C14H28Z+R3OOH=>R2OH+C14H28OE#3    1.0E+0012  0.000  14200.0  ! ADZ 494

!   olefin to dienes
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    5.4E+0004  2.500  -1900.0  ! MZ 495
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    2.9E+0007  2.000  7700.0  ! MZ 496
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    9.0E+0006  2.000  5000.0  ! MZ 497
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    3.0E+0006  2.000  -1520.0  ! MZ 498
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.7E+0006  2.000  450.0  ! MZ 499
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.6E+0006  2.000  -765.0  ! MZ 500
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.4E+0003  2.600  12400.0  ! MZ 501
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.0E+0011  0.000  17000.0  ! MZ 502
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    4.0E+0011  0.000  15500.0  ! MZ 503
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    1.0E+0011  0.000  7300.0  ! MZ 504
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    3.0E-0001  4.000  8200.0  ! MZ 505
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    2.0E+0011  0.000  9600.0  ! MZ 506
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    1.0E+0012  0.000  14550.0  ! MZ
507
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     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    6.0E+0012  0.000  20000.0  ! MZ
508
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    3.0E+0012  0.000  17500.0  ! MZ
509
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    1.5E+0000  3.500  4140.0  ! MZ 510
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    3.0E+0011  0.000  13500.0  ! MZ 511
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    2.0E+0011  0.000  11000.0  ! MZ 512
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    5.4E+0004  2.500  -1900.0  ! MZ 513
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.9E+0007  2.000  7700.0  ! MZ 514
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.7E+0007  2.000  5000.0  ! MZ 515
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    3.0E+0006  2.000  -1520.0  ! MZ 516
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    2.7E+0006  2.000  450.0  ! MZ 517
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    7.8E+0006  2.000  -765.0  ! MZ 518
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.4E+0003  2.600  12400.0  ! MZ 519
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.0E+0011  0.000  17000.0  ! MZ 520
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    1.2E+0012  0.000  15500.0  ! MZ 521
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    1.0E+0011  0.000  7300.0  ! MZ 522
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    3.0E-0001  4.000  8200.0  ! MZ 523
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    6.0E+0011  0.000  9600.0  ! MZ 524
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    1.0E+0012  0.000  14550.0  ! MZ
525
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    6.0E+0012  0.000  20000.0  ! MZ
526
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    9.0E+0012  0.000  17500.0  ! MZ
527
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    1.5E+0000  3.500  4140.0  ! MZ 528
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    3.0E+0011  0.000  13500.0  ! MZ
529
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    6.0E+0011  0.000  11000.0  ! MZ
530
     DUPLICATE
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C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    5.4E+0004  2.500  -1900.0  ! MZ 531
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    2.9E+0007  2.000  7700.0  ! MZ 532
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    1.8E+0007  2.000  5000.0  ! MZ 533
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    3.0E+0006  2.000  -1520.0  ! MZ 534
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    2.7E+0006  2.000  450.0  ! MZ 535
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    5.2E+0006  2.000  -765.0  ! MZ 536
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.4E+0003  2.600  12400.0  ! MZ 537
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.0E+0011  0.000  17000.0  ! MZ 538
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    8.0E+0011  0.000  15500.0  ! MZ 539
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    1.0E+0011  0.000  7300.0  ! MZ 540
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    3.0E-0001  4.000  8200.0  ! MZ 541
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    4.0E+0011  0.000  9600.0  ! MZ 542
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    1.0E+0012  0.000  14550.0  ! MZ
543
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  20000.0  ! MZ
544
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  17500.0  ! MZ
545
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    1.5E+0000  3.500  4140.0  ! MZ 546
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    3.0E+0011  0.000  13500.0  ! MZ
547
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    4.0E+0011  0.000  11000.0  ! MZ
548
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    5.4E+0004  2.500  -1900.0  ! MZ 549
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    2.9E+0007  2.000  7700.0  ! MZ 550
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    3.6E+0007  2.000  5000.0  ! MZ 551
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    3.0E+0006  2.000  -1520.0  ! MZ 552
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    2.7E+0006  2.000  450.0  ! MZ 553
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    1.0E+0007  2.000  -765.0  ! MZ 554
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.4E+0003  2.600  12400.0  ! MZ 555
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     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.0E+0011  0.000  17000.0  ! MZ 556
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    1.6E+0012  0.000  15500.0  ! MZ 557
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    1.0E+0011  0.000  7300.0  ! MZ 558
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    3.0E-0001  4.000  8200.0  ! MZ 559
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    8.0E+0011  0.000  9600.0  ! MZ 560
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.0E+0012  0.000  14550.0  ! MZ
561
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    6.0E+0012  0.000  20000.0  ! MZ
562
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.2E+0013  0.000  17500.0  ! MZ
563
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    1.5E+0000  3.500  4140.0  ! MZ 564
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    3.0E+0011  0.000  13500.0  ! MZ
565
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    8.0E+0011  0.000  11000.0  ! MZ
566
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    5.4E+0004  2.500  -1900.0  ! MZ 567
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    2.9E+0007  2.000  7700.0  ! MZ 568
     DUPLICATE
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    4.5E+0007  2.000  5000.0  ! MZ 569
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    3.0E+0006  2.000  -1520.0  ! MZ 570
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    2.7E+0006  2.000  450.0  ! MZ 571
     DUPLICATE
C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    1.3E+0007  2.000  -765.0  ! MZ 572
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.4E+0003  2.600  12400.0  ! MZ 573
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.0E+0011  0.000  17000.0  ! MZ 574
     DUPLICATE
C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    2.0E+0012  0.000  15500.0  ! MZ 575
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0011  0.000  7300.0  ! MZ 576
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    3.0E-0001  4.000  8200.0  ! MZ 577
     DUPLICATE
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0012  0.000  9600.0  ! MZ 578
     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.0E+0012  0.000  14550.0  ! MZ
579
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     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    6.0E+0012  0.000  20000.0  ! MZ
580
     DUPLICATE
C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.5E+0013  0.000  17500.0  ! MZ
581
     DUPLICATE
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.5E+0000  3.500  4140.0  ! MZ
582
     DUPLICATE
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    3.0E+0011  0.000  13500.0  ! MZ
583
     DUPLICATE
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.0E+0012  0.000  11000.0  ! MZ
584
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0004  2.500  -1900.0  ! MZ 585
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    2.9E+0007  2.000  7700.0  ! MZ 586
     DUPLICATE
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0007  2.000  5000.0  ! MZ 587
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    3.0E+0006  2.000  -1520.0  ! MZ 588
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    2.7E+0006  2.000  450.0  ! MZ 589
     DUPLICATE
C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    1.5E+0007  2.000  -765.0  ! MZ 590
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.4E+0003  2.600  12400.0  ! MZ
591
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.0E+0011  0.000  17000.0  ! MZ
592
     DUPLICATE
C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    2.4E+0012  0.000  15500.0  ! MZ
593
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.0E+0011  0.000  7300.0  ! MZ 594
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    3.0E-0001  4.000  8200.0  ! MZ 595
     DUPLICATE
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.2E+0012  0.000  9600.0  ! MZ 596
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.0E+0012  0.000  14550.0  !
MZ 597
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    6.0E+0012  0.000  20000.0  !
MZ 598
     DUPLICATE
C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.8E+0013  0.000  17500.0  !
MZ 599
     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.5E+0000  3.500  4140.0  ! MZ
600
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     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    3.0E+0011  0.000  13500.0  ! MZ
601
     DUPLICATE
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.2E+0012  0.000  11000.0  ! MZ
602
     DUPLICATE
!C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
603
!C13H26Z+R2OH=>H2O+C4H6Z2+R4CH3+4C2H4Z    3.0E+0006  2.000  -1520.0  ! MZ
604
!C13H26Z+R3OOH=>H2O2+C4H6Z2+R4CH3+4C2H4Z    6.4E+0003  2.600  12400.0  !
MZ 605
!C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0  ! MZ
606
!C13H26Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0
! MZ 607
!C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z    1.5E+0000  3.500  4140.0  !
MZ 608
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    5.4E+0004  2.500  -1900.0  ! MZ 609
     DUPLICATE
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    2.9E+0007  2.000  7700.0  ! MZ 610
     DUPLICATE
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    7.2E+0007  2.000  5000.0  ! MZ 611
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    3.0E+0006  2.000  -1520.0  ! MZ 612
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.7E+0006  2.000  450.0  ! MZ 613
     DUPLICATE
C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.1E+0007  2.000  -765.0  ! MZ 614
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.4E+0003  2.600  12400.0  ! MZ
615
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.0E+0011  0.000  17000.0  ! MZ
616
     DUPLICATE
C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    3.2E+0012  0.000  15500.0  ! MZ
617
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.0E+0011  0.000  7300.0  ! MZ 618
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    3.0E-0001  4.000  8200.0  ! MZ 619
     DUPLICATE
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.6E+0012  0.000  9600.0  ! MZ 620
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    1.0E+0012  0.000  14550.0  !
MZ 621
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    6.0E+0012  0.000  20000.0  !
MZ 622
     DUPLICATE
C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    2.4E+0013  0.000  17500.0  !
MZ 623
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     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.5E+0000  3.500  4140.0  ! MZ
624
     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    3.0E+0011  0.000  13500.0  ! MZ
625
     DUPLICATE
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.6E+0012  0.000  11000.0  ! MZ
626
     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    5.4E+0004  2.500  -1900.0  ! MZ 627
     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    2.9E+0007  2.000  7700.0  ! MZ 628
     DUPLICATE
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    6.3E+0007  2.000  5000.0  ! MZ 629
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    3.0E+0006  2.000  -1520.0  ! MZ 630
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    2.7E+0006  2.000  450.0  ! MZ 631
     DUPLICATE
C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    1.8E+0007  2.000  -765.0  ! MZ 632
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.4E+0003  2.600  12400.0  ! MZ
633
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.0E+0011  0.000  17000.0  ! MZ
634
     DUPLICATE
C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    2.8E+0012  0.000  15500.0  ! MZ
635
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.0E+0011  0.000  7300.0  ! MZ 636
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    3.0E-0001  4.000  8200.0  ! MZ 637
     DUPLICATE
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.4E+0012  0.000  9600.0  ! MZ 638
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    1.0E+0012  0.000  14550.0  !
MZ 639
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    6.0E+0012  0.000  20000.0  !
MZ 640
     DUPLICATE
C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    2.1E+0013  0.000  17500.0  !
MZ 641
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.5E+0000  3.500  4140.0  ! MZ
642
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    3.0E+0011  0.000  13500.0  ! MZ
643
     DUPLICATE
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.4E+0012  0.000  11000.0  ! MZ
644
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     DUPLICATE
!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
645
!C14H28Z+R2OH=>H2O+C4H6Z2+R11C2H5+4C2H4Z    3.0E+0006  2.000  -1520.0  !
MZ 646
!C14H28Z+R3OOH=>H2O2+C4H6Z2+R11C2H5+4C2H4Z    6.4E+0003  2.600
12400.0  ! MZ 647
!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000  7300.0  !
MZ 648
!C14H28Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000
7300.0  ! MZ 649
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z    1.5E+0000  3.500  4140.0
! MZ 650
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    8.8E+0010  0.700  3250.0  ! MZ 651
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    5.1E+0013  0.000  7850.0  ! MZ 652
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    2.6E+0013  0.000  5200.0  ! MZ 653
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    8.8E+0010  0.700  3250.0  ! MZ 654
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    5.1E+0013  0.000  7850.0  ! MZ 655
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    7.8E+0013  0.000  5200.0  ! MZ 656
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    8.8E+0010  0.700  3250.0  ! MZ 657
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.1E+0013  0.000  7850.0  ! MZ 658
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.2E+0013  0.000  5200.0  ! MZ 659
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    8.8E+0010  0.700  3250.0  ! MZ 660
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    5.1E+0013  0.000  7850.0  ! MZ 661
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    1.0E+0014  0.000  5200.0  ! MZ 662
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    8.8E+0010  0.700  3250.0  ! MZ 663
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    5.1E+0013  0.000  7850.0  ! MZ 664
     DUPLICATE
C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    1.3E+0014  0.000  5200.0  ! MZ 665
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    8.8E+0010  0.700  3250.0  ! MZ 666
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    5.1E+0013  0.000  7850.0  ! MZ 667
     DUPLICATE
C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    1.6E+0014  0.000  5200.0  ! MZ 668
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    8.8E+0010  0.700  3250.0  ! MZ 669
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    5.1E+0013  0.000  7850.0  ! MZ 670
     DUPLICATE
C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    2.1E+0014  0.000  5200.0  ! MZ 671
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     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    8.8E+0010  0.700  3250.0  ! MZ 672
     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    5.1E+0013  0.000  7850.0  ! MZ 673
     DUPLICATE
C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    1.8E+0014  0.000  5200.0  ! MZ 674
     DUPLICATE

! Metathesis with YH
C3H6Y+R1H=>RC3H5Y+H2    1.7E+0005  2.500  2510.0  ! MES 675
C3H6Y+R2OH=>RC3H5Y+H2O    3.0E+0006  2.000  -298.0  ! MES 676
C3H6Y+R3OOH=>RC3H5Y+H2O2    9.6E+0003  2.600  13900.0  ! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4    2.2E+0000  3.500  5670.0  ! MES 678
C3H6Y+R8CH3OO=>RC3H5Y+CH3OOH    2.0E+0012  0.000  17050.0  ! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6    2.2E+0000  3.500  6640.0  ! MES 680
C4H8Y+R1H=>RC4H7Y+H2    5.4E+0004  2.500  -1900.0  ! MES 681
     DUPLICATE
C4H8Y+R1H=>RC4H7Y+H2    2.9E+0007  2.000  7700.0  ! MES 682
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 683
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    2.7E+0006  2.000  450.0  ! MES 684
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 685
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 686
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    1.0E+0011  0.000  7300.0  ! MES 687
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    3.0E-0001  4.000  8200.0  ! MES 688
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 689
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 690
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 691
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 692
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    5.4E+0004  2.500  -1900.0  ! MES 693
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.9E+0007  2.000  7700.0  ! MES 694
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.7E+0007  2.000  5000.0  ! MES 695
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 696
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    2.7E+0006  2.000  450.0  ! MES 697
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    7.8E+0006  2.000  -765.0  ! MES 698
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 699
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 700
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     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    1.2E+0012  0.000  15500.0  ! MES 701
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    1.0E+0011  0.000  7300.0  ! MES 702
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    3.0E-0001  4.000  8200.0  ! MES 703
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    6.0E+0011  0.000  9600.0  ! MES 704
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 705
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 706
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    9.0E+0012  0.000  17500.0  ! MES 707
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 708
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 709
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    6.0E+0011  0.000  11000.0  ! MES 710
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    5.4E+0004  2.500  -1900.0  ! MES 711
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    2.9E+0007  2.000  7700.0  ! MES 712
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    3.6E+0007  2.000  5000.0  ! MES 713
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 714
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    2.7E+0006  2.000  450.0  ! MES 715
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    1.0E+0007  2.000  -765.0  ! MES 716
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 717
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 718
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    1.6E+0012  0.000  15500.0  ! MES 719
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    1.0E+0011  0.000  7300.0  ! MES 720
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    3.0E-0001  4.000  8200.0  ! MES 721
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    8.0E+0011  0.000  9600.0  ! MES 722
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 723
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 724
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.2E+0013  0.000  17500.0  ! MES 725
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 726
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 727
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     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    8.0E+0011  0.000  11000.0  ! MES 728
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    5.4E+0004  2.500  -1900.0  ! MES 729
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    2.9E+0007  2.000  7700.0  ! MES 730
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    9.0E+0006  2.000  5000.0  ! MES 731
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 732
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.7E+0006  2.000  450.0  ! MES 733
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.6E+0006  2.000  -765.0  ! MES 734
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 735
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 736
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    4.0E+0011  0.000  15500.0  ! MES 737
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    1.0E+0011  0.000  7300.0  ! MES 738
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    3.0E-0001  4.000  8200.0  ! MES 739
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    2.0E+0011  0.000  9600.0  ! MES 740
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 741
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 742
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    3.0E+0012  0.000  17500.0  ! MES 743
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 744
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 745
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    2.0E+0011  0.000  11000.0  ! MES 746
     DUPLICATE
C3H6Y+B1O=>RC3H5Y+R2OH    1.7E+0011  0.700  5900.0  ! MES 747
C4H8Y+B1O=>RC4H7Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 748
     DUPLICATE
C4H8Y+B1O=>RC4H7Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 749
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 750
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 751
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    7.8E+0013  0.000  5200.0  ! MES 752
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 753
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 754
     DUPLICATE
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C8H16Y+B1O=>RC8H15Y+R2OH    1.0E+0014  0.000  5200.0  ! MES 755
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 756
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 757
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    2.6E+0013  0.000  5200.0  ! MES 758
     DUPLICATE

! Addition of .Y on YH
RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 759
RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 760
RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 761
RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 762
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y    6.0E+0009  0.000  11400.0  ! ADY 763
RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 764
RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 765
RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 766
RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 767
RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 768
RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 769
RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 770
RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z    6.0E+0009  0.000  11400.0  ! ADY 771
RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 772
RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 773
RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 774
!RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z    6.0E+0009  0.000  11400.0  ! ADY 775
RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 776
RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 777
RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 778
RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 779
RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 780
RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 781
RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 782
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 783

! Alkohol reactions
C3H7OH+R1H=>H2+R2OH+C3H6Y    2.9E+0007  2.000  7700.0  ! MOL 784
     DUPLICATE
C3H7OH+R1H=>H2+R2OH+C3H6Y    1.8E+0007  2.000  5000.0  ! MOL 785
     DUPLICATE
C3H7OH+R1H=>H2+R11C2H5+HCHO    2.4E+0006  2.000  6525.0  ! MOL 786
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    2.7E+0006  2.000  450.0  ! MOL 787
     DUPLICATE
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    5.2E+0006  2.000  -765.0  ! MOL 788
     DUPLICATE
C3H7OH+R2OH=>H2O+R11C2H5+HCHO    4.0E+0005  2.000  -475.0  ! MOL 789
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    6.0E+0011  0.000  17000.0  ! MOL 790
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    8.0E+0011  0.000  15500.0  ! MOL 791
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R11C2H5+HCHO    5.4E+0004  2.000  15025.0  ! MOL 792
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    3.0E-0001  4.000  8200.0  ! MOL 793
     DUPLICATE
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C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    4.0E+0011  0.000  9600.0  ! MOL 794
     DUPLICATE
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO    3.9E+0004  2.000  7525.0  ! MOL 795
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    1.6E+0011  0.000  7300.0  ! MOL 796
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    2.9E+0011  0.000  4500.0  ! MOL 797
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R11C2H5+HCHO    0.0E+0000  0.000  0.0  ! MOL 798
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    3.0E+0011  0.000  13500.0  ! MOL 799
     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    4.0E+0011  0.000  11000.0  ! MOL 800
     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R11C2H5+HCHO    2.3E+0004  2.000  10525.0  ! MOL 801
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.9E+0007  2.000  7700.0  ! MOL 802
     DUPLICATE
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.7E+0007  2.000  5000.0  ! MOL 803
     DUPLICATE
C4H10OL+R1H=>H2+R19C3H7+HCHO    2.4E+0006  2.000  6525.0  ! MOL 804
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    2.7E+0006  2.000  450.0  ! MOL 805
     DUPLICATE
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    7.8E+0006  2.000  -765.0  ! MOL 806
     DUPLICATE
C4H10OL+R2OH=>H2O+R19C3H7+HCHO    4.0E+0005  2.000  -475.0  ! MOL 807
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    6.0E+0011  0.000  17000.0  ! MOL 808
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    1.2E+0012  0.000  15500.0  ! MOL 809
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R19C3H7+HCHO    5.4E+0004  2.000  15025.0  ! MOL 810
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    3.0E-0001  4.000  8200.0  ! MOL 811
     DUPLICATE
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    6.0E+0011  0.000  9600.0  ! MOL 812
     DUPLICATE
C4H10OL+R4CH3=>CH4+R19C3H7+HCHO    3.9E+0004  2.000  7525.0  ! MOL 813
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    1.6E+0011  0.000  7300.0  ! MOL 814
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    4.4E+0011  0.000  4500.0  ! MOL 815
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R19C3H7+HCHO    0.0E+0000  0.000  0.0  ! MOL 816
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    3.0E+0011  0.000  13500.0  ! MOL 817
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    6.0E+0011  0.000  11000.0  ! MOL 818
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R19C3H7+HCHO    2.3E+0004  2.000  10525.0  ! MOL
819
C5H12OL+R1H=>H2+R2OH+C5H10Z    2.9E+0007  2.000  7700.0  ! MOL 820
     DUPLICATE
C5H12OL+R1H=>H2+R2OH+C5H10Z    3.6E+0007  2.000  5000.0  ! MOL 821
     DUPLICATE
C5H12OL+R1H=>H2+R20C4H9+HCHO    2.4E+0006  2.000  6525.0  ! MOL 822
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    2.7E+0006  2.000  450.0  ! MOL 823
     DUPLICATE
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    1.0E+0007  2.000  -765.0  ! MOL 824
     DUPLICATE
C5H12OL+R2OH=>H2O+R20C4H9+HCHO    4.0E+0005  2.000  -475.0  ! MOL 825
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C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    6.0E+0011  0.000  17000.0  ! MOL 826
     DUPLICATE
C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    1.6E+0012  0.000  15500.0  ! MOL 827
     DUPLICATE
C5H12OL+R3OOH=>H2O2+R20C4H9+HCHO    5.4E+0004  2.000  15025.0  ! MOL 828
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    3.0E-0001  4.000  8200.0  ! MOL 829
     DUPLICATE
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    8.0E+0011  0.000  9600.0  ! MOL 830
     DUPLICATE
C5H12OL+R4CH3=>CH4+R20C4H9+HCHO    3.9E+0004  2.000  7525.0  ! MOL 831
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    1.6E+0011  0.000  7300.0  ! MOL
832
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    5.8E+0011  0.000  4500.0  ! MOL
833
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R20C4H9+HCHO    0.0E+0000  0.000  0.0  ! MOL 834
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    3.0E+0011  0.000  13500.0  ! MOL 835
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    8.0E+0011  0.000  11000.0  ! MOL 836
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R20C4H9+HCHO    2.3E+0004  2.000  10525.0  ! MOL
837
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    3.9E+0013  0.000  5200.0  ! MOL 838
     DUPLICATE
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    4.0E+0013  0.000  5200.0  ! MOL 839
     DUPLICATE
C3H7OH+B1O=>R2OH+R11C2H5+HCHO    1.3E+0006  2.000  5025.0  ! MOL 840
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    3.9E+0013  0.000  5200.0  ! MOL 841
     DUPLICATE
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    6.0E+0013  0.000  5200.0  ! MOL 842
     DUPLICATE
C4H10OL+B1O=>R2OH+R19C3H7+HCHO    1.3E+0006  2.000  5025.0  ! MOL 843
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    3.9E+0013  0.000  5200.0  ! MOL 844
     DUPLICATE
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    8.0E+0013  0.000  5200.0  ! MOL 845
     DUPLICATE
C5H12OL+B1O=>R2OH+R20C4H9+HCHO    1.3E+0006  2.000  5025.0  ! MOL 846

! Aldehydes metathesis
C2H5CHO+R1H=>H2+RC3H5O    4.0E+0013  0.000  4200.0  ! ADZ 847
C2H5CHO+R2OH=>H2O+RC3H5O    4.2E+0012  0.000  500.0  ! ADZ 848
C2H5CHO+R3OOH=>H2O2+RC3H5O    1.0E+0012  0.000  10000.0  ! ADZ 849
C2H5CHO+R4CH3=>CH4+RC3H5O    2.0E-0006  5.600  2500.0  ! ADZ 850
C2H5CHO+R11C2H5=>C2H6+RC3H5O    1.3E+0012  0.000  8500.0  ! ADZ 851
C5H10OA+R1H=>H2+RC5H9O    4.0E+0013  0.000  4200.0  ! ADZ 852
C5H10OA+R2OH=>H2O+RC5H9O    4.2E+0012  0.000  500.0  ! ADZ 853
C5H10OA+R3OOH=>H2O2+RC5H9O    1.0E+0012  0.000  10000.0  ! ADZ 854
C5H10OA+R4CH3=>CH4+RC5H9O    2.0E-0006  5.600  2500.0  ! ADZ 855
C5H10OA+R11C2H5=>C2H6+RC5H9O    1.3E+0012  0.000  8500.0  ! ADZ 856
C4H8OA+R1H=>H2+RC4H7O    4.0E+0013  0.000  4200.0  ! ADZ 857
C4H8OA+R2OH=>H2O+RC4H7O    4.2E+0012  0.000  500.0  ! ADZ 858
C4H8OA+R3OOH=>H2O2+RC4H7O    1.0E+0012  0.000  10000.0  ! ADZ 859
C4H8OA+R4CH3=>CH4+RC4H7O    2.0E-0006  5.600  2500.0  ! ADZ 860
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C4H8OA+R11C2H5=>C2H6+RC4H7O    1.3E+0012  0.000  8500.0  ! ADZ 861
C6H12OA+R1H=>H2+RC6H11O    4.0E+0013  0.000  4200.0  ! ADZ 862
C6H12OA+R2OH=>H2O+RC6H11O    4.2E+0012  0.000  500.0  ! ADZ 863
C6H12OA+R3OOH=>H2O2+RC6H11O    1.0E+0012  0.000  10000.0  ! ADZ 864
C6H12OA+R4CH3=>CH4+RC6H11O    2.0E-0006  5.600  2500.0  ! ADZ 865
C6H12OA+R11C2H5=>C2H6+RC6H11O    1.3E+0012  0.000  8500.0  ! ADZ 866
C7H14OA+R1H=>H2+RC7H13O    4.0E+0013  0.000  4200.0  ! ADZ 867
C7H14OA+R2OH=>H2O+RC7H13O    4.2E+0012  0.000  500.0  ! ADZ 868
C7H14OA+R3OOH=>H2O2+RC7H13O    1.0E+0012  0.000  10000.0  ! ADZ 869
C7H14OA+R4CH3=>CH4+RC7H13O    2.0E-0006  5.600  2500.0  ! ADZ 870
C7H14OA+R11C2H5=>C2H6+RC7H13O    1.3E+0012  0.000  8500.0  ! ADZ 871
C8H16OA+R1H=>H2+RC8H15O    4.0E+0013  0.000  4200.0  ! ADZ 872
C8H16OA+R2OH=>H2O+RC8H15O    4.2E+0012  0.000  500.0  ! ADZ 873
C8H16OA+R3OOH=>H2O2+RC8H15O    1.0E+0012  0.000  10000.0  ! ADZ 874
C8H16OA+R4CH3=>CH4+RC8H15O    2.0E-0006  5.600  2500.0  ! ADZ 875
C8H16OA+R11C2H5=>C2H6+RC8H15O    1.3E+0012  0.000  8500.0  ! ADZ 876
C9H18OA+R1H=>H2+RC9H17O    4.0E+0013  0.000  4200.0  ! ADZ 877
C9H18OA+R2OH=>H2O+RC9H17O    4.2E+0012  0.000  500.0  ! ADZ 878
C9H18OA+R3OOH=>H2O2+RC9H17O    1.0E+0012  0.000  10000.0  ! ADZ 879
C9H18OA+R4CH3=>CH4+RC9H17O    2.0E-0006  5.600  2500.0  ! ADZ 880
C9H18OA+R11C2H5=>C2H6+RC9H17O    1.3E+0012  0.000  8500.0  ! ADZ 881
C12H24OA+R1H=>H2+RC12H23O    4.0E+0013  0.000  4200.0  ! ADZ 882
C12H24OA+R2OH=>H2O+RC12H23O    4.2E+0012  0.000  500.0  ! ADZ 883
C12H24OA+R3OOH=>H2O2+RC12H23O    1.0E+0012  0.000  10000.0  ! ADZ 884
C12H24OA+R4CH3=>CH4+RC12H23O    2.0E-0006  5.600  2500.0  ! ADZ 885
C12H24OA+R11C2H5=>C2H6+RC12H23O    1.3E+0012  0.000  8500.0  ! ADZ 886
C11H22OA+R1H=>H2+RC11H21O    4.0E+0013  0.000  4200.0  ! ADZ 887
C11H22OA+R2OH=>H2O+RC11H21O    4.2E+0012  0.000  500.0  ! ADZ 888
C11H22OA+R3OOH=>H2O2+RC11H21O    1.0E+0012  0.000  10000.0  ! ADZ 889
C11H22OA+R4CH3=>CH4+RC11H21O    2.0E-0006  5.600  2500.0  ! ADZ 890
C11H22OA+R11C2H5=>C2H6+RC11H21O    1.3E+0012  0.000  8500.0  ! ADZ 891
C10H20OA+R1H=>H2+RC10H19O    4.0E+0013  0.000  4200.0  ! ADZ 892
C10H20OA+R2OH=>H2O+RC10H19O    4.2E+0012  0.000  500.0  ! ADZ 893
C10H20OA+R3OOH=>H2O2+RC10H19O    1.0E+0012  0.000  10000.0  ! ADZ 894
C10H20OA+R4CH3=>CH4+RC10H19O    2.0E-0006  5.600  2500.0  ! ADZ 895
C10H20OA+R11C2H5=>C2H6+RC10H19O    1.3E+0012  0.000  8500.0  ! ADZ 896
C13H26OA+R1H=>H2+RC13H25O    4.0E+0013  0.000  4200.0  ! ADZ 897
C13H26OA+R2OH=>H2O+RC13H25O    4.2E+0012  0.000  500.0  ! ADZ 898
C13H26OA+R3OOH=>H2O2+RC13H25O    1.0E+0012  0.000  10000.0  ! ADZ 899
C13H26OA+R4CH3=>CH4+RC13H25O    2.0E-0006  5.600  2500.0  ! ADZ 900
C13H26OA+R11C2H5=>C2H6+RC13H25O    1.3E+0012  0.000  8500.0  ! ADZ 901

C4H6OAY+R1H=>H2+R10C2H3V+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 902
C4H6OAY+R2OH=>H2O+R10C2H3V+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 903
C4H6OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ
904
C4H6OAY+R4CH3=>CH4+R10C2H3V+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 905
C4H6OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
906
C5H8OAY+R1H=>H2+RC3H5Y+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 907
C5H8OAY+R2OH=>H2O+RC3H5Y+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 908
C5H8OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ 909
C5H8OAY+R4CH3=>CH4+RC3H5Y+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 910
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C5H8OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
911
!C8H14OAY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 912
!C8H14OAY+R2OH=>H2O+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 913
!C8H14OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+2C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 914
!C8H14OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z    2.0E-0006  0.000
2500.0  ! ADZ 915
!C8H14OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z    1.3E+0012  0.000
8500.0  ! ADZ 916
!C9H16OAY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  ! ADZ
917
!C9H16OAY+R2OH=>H2O+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 918
!C9H16OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ+2C2H4Z    1.0E+0012  0.000
10000.0  ! ADZ 919
!C9H16OAY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 920
!C9H16OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 921
!C6H10OAY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 922
!C6H10OAY+R2OH=>H2O+R10C2H3V+CH2COZ+C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 923
!C6H10OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 924
!C6H10OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 925
!C6H10OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 926

! Keto radicals decomposition
RC3H5O=>B2CO+R11C2H5    1.8E+0014  0.000  15600.0  ! COR 927
RC5H9O=>B2CO+R20C4H9    1.8E+0014  0.000  15600.0  ! COR 928
RC4H7O=>B2CO+R19C3H7    1.8E+0014  0.000  15600.0  ! COR 929
RC6H11O=>B2CO+R35C5H11    1.8E+0014  0.000  15600.0  ! COR 930
RC7H13O=>B2CO+R41C6H13    1.8E+0014  0.000  15600.0  ! COR 931
RC8H15O=>B2CO+R26C7H15    1.8E+0014  0.000  15600.0  ! COR 932
RC9H17O=>B2CO+R30C8H17    1.8E+0014  0.000  15600.0  ! COR 933
RC12H23O=>B2CO+R4CH3+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 934
RC11H21O=>B2CO+R11C2H5+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 935
RC10H19O=>B2CO+R4CH3+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 936
RC13H25O=>B2CO+R11C2H5+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 937


! keto radicals addition to O2
RC3H5O+O2=>RC3H5O3    3.0E+0019  -2.500  0.0  ! COR 938
RC5H9O+O2=>RC5H9O3    3.0E+0019  -2.500  0.0  ! COR 939
RC4H7O+O2=>RC4H7O3    3.0E+0019  -2.500  0.0  ! COR 940
RC6H11O+O2=>RC6H11O3    3.0E+0019  -2.500  0.0  ! COR 941
RC7H13O+O2=>RC7H13O3    3.0E+0019  -2.500  0.0  ! COR 942
RC8H15O+O2=>RC8H15O3    3.0E+0019  -2.500  0.0  ! COR 943
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RC9H17O+O2=>RC9H17O3    3.0E+0019  -2.500  0.0  ! COR 944
RC12H23O+O2=>RC12H23O3    3.0E+0019  -2.500  0.0  ! COR 945
RC11H21O+O2=>RC11H21O3    3.0E+0019  -2.500  0.0  ! COR 946
RC10H19O+O2=>RC10H19O3    3.0E+0019  -2.500  0.0  ! COR 947
RC13H25O+O2=>RC13H25O3    3.0E+0019  -2.500  0.0  ! COR 948

! Peracide radical decomposition
RC3H5O3=>C2H4Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 949
RC5H9O3=>C4H8Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 950
RC4H7O3=>C3H6Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 951
RC6H11O3=>C5H10Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 952
RC7H13O3=>C6H12Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 953
RC8H15O3=>C7H14Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 954
RC9H17O3=>C8H16Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 955
RC12H23O3=>C11H22Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 956
RC11H21O3=>C10H20Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 957
RC10H19O3=>C9H18Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 958
RC13H25O3=>C12H24Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 959

! Ketones reactions
!C2H6CO+R1H=>H2+CH2COZ+R4CH3    5.7E+0007  2.000  7700.0  ! MK 960
!C2H6CO+R2OH=>H2O+CH2COZ+R4CH3    5.4E+0006  2.000  450.0  ! MK 961
!C2H6CO+R3OOH=>H2O2+CH2COZ+R4CH3    1.2E+0012  0.000  17000.0  ! MK 962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3    6.0E-0001  4.000  8200.0  ! MK 963
!C2H6CO+R8CH3OO=>CH3OOH+CH2COZ+R4CH3    1.2E+0013  0.000  20000.0  ! MK
964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3    6.0E+0011  0.000  13500.0  ! MK 965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    5.7E+0007  2.000  7700.0  ! MK 966
     DUPLICATE
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    9.0E+0006  2.000  5000.0  ! MK 967
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    5.4E+0006  2.000  450.0  ! MK 968
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    2.6E+0006  2.000  -765.0  ! MK 969
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    1.2E+0012  0.000  17000.0  ! MK 970
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    4.0E+0011  0.000  15500.0  ! MK 971
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    6.0E-0001  4.000  8200.0  ! MK 972
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    2.0E+0011  0.000  9600.0  ! MK 973
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    1.2E+0013  0.000  20000.0  ! MK
974
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    3.0E+0012  0.000  17500.0  ! MK
975
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    6.0E+0011  0.000  13500.0  ! MK
976
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    2.0E+0011  0.000  11000.0  ! MK
977
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DUPLICATE

! Unsaturated ester reactions
! Esters metatesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis
! Addition on unsaturated esters

! Carboxylic acid reactions
! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alkohol ene to dienes
C3H6OLY+R1H=>H2+HCHO+R10C2H3V 5.4E+0004 2.500 -1900.0 ! ROH 978
C3H6OLY+R2OH=>H2O+HCHO+R10C2H3V 3.0E+0006 2.000 -1520.0 ! ROH 979
C3H6OLY+R3OOH=>H2O2+HCHO+R10C2H3V 6.4E+0003 2.600 12400.0 ! ROH 980
C3H6OLY+R4CH3=>CH4+HCHO+R10C2H3V 1.0E+0011 0.000 7300.0 ! ROH 981
C3H6OLY+R8CH3OO=>CH3OOH+HCHO+R10C2H3V 1.0E+0012 0.000 14550.0 ! ROH 982
C3H6OLY+R11C2H5=>C2H6+HCHO+R10C2H3V 1.5E+0000 3.500 4140.0 ! ROH 983
C4H8OLY+R1H=>H2+HCHO+RC3H5Y 5.4E+0004 2.500 -1900.0 ! ROH 984
C4H8OLY+R2OH=>H2O+HCHO+RC3H5Y 3.0E+0006 2.000 -1520.0 ! ROH 985
C4H8OLY+R3OOH=>H2O2+HCHO+RC3H5Y 6.4E+0003 2.600 12400.0 ! ROH 986
C4H8OLY+R4CH3=>CH4+HCHO+RC3H5Y 1.0E+0011 0.000 7300.0 ! ROH 987
C4H8OLY+R8CH3OO=>CH3OOH+HCHO+RC3H5Y 1.0E+0012 0.000 14550.0 ! ROH 988
C4H8OLY+R11C2H5=>C2H6+HCHO+RC3H5Y 1.5E+0000 3.500 4140.0 ! ROH 989
C5H10OLY+R1H=>H2+HCHO+RC4H7Y 5.4E+0004 2.500 -1900.0 ! ROH 990
C5H10OLY+R2OH=>H2O+HCHO+RC4H7Y 3.0E+0006 2.000 -1520.0 ! ROH 991
C5H10OLY+R3OOH=>H2O2+HCHO+RC4H7Y 6.4E+0003 2.600 12400.0 ! ROH 992
C5H10OLY+R4CH3=>CH4+HCHO+RC4H7Y 1.0E+0011 0.000 7300.0 ! ROH 993
C5H10OLY+R8CH3OO=>CH3OOH+HCHO+RC4H7Y 1.0E+0012 0.000 14550.0 ! ROH 994
C5H10OLY+R11C2H5=>C2H6+HCHO+RC4H7Y 1.5E+0000 3.500 4140.0 ! ROH 995
C7H14OLY+R1H=>H2+HCHO+RC6H11Y 5.4E+0004 2.500 -1900.0 ! ROH 996
C7H14OLY+R2OH=>H2O+HCHO+RC6H11Y 3.0E+0006 2.000 -1520.0 ! ROH 997
C7H14OLY+R3OOH=>H2O2+HCHO+RC6H11Y 6.4E+0003 2.600 12400.0 ! ROH 998
C7H14OLY+R4CH3=>CH4+HCHO+RC6H11Y 1.0E+0011 0.000 7300.0 ! ROH 999
C7H14OLY+R8CH3OO=>CH3OOH+HCHO+RC6H11Y 1.0E+0012 0.000 14550.0 ! ROH 1000
C7H14OLY+R11C2H5=>C2H6+HCHO+RC6H11Y 1.5E+0000 3.500 4140.0 ! ROH 1001
C8H16OLY+R1H=>H2+HCHO+RC7H13Y 5.4E+0004 2.500 -1900.0 ! ROH 1002
C8H16OLY+R2OH=>H2O+HCHO+RC7H13Y 3.0E+0006 2.000 -1520.0 ! ROH 1003
C8H16OLY+R3OOH=>H2O2+HCHO+RC7H13Y 6.4E+0003 2.600 12400.0 ! ROH 1004
C8H16OLY+R4CH3=>CH4+HCHO+RC7H13Y 1.0E+0011 0.000 7300.0 ! ROH 1005

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C8H16OLY+R8CH3OO=>CH3OOH+HCHO+RC7H13Y    1.0E+0012  0.000  14550.0  ! ROH
1006
C8H16OLY+R11C2H5=>C2H6+HCHO+RC7H13Y    1.5E+0000  3.500  4140.0  ! ROH
1007
C9H18OLY+R1H=>H2+HCHO+RC8H15Y    5.4E+0004  2.500  -1900.0  ! ROH 1008
C9H18OLY+R2OH=>H2O+HCHO+RC8H15Y    3.0E+0006  2.000  -1520.0  ! ROH 1009
C9H18OLY+R3OOH=>H2O2+HCHO+RC8H15Y    6.4E+0003  2.600  12400.0  ! ROH
1010
C9H18OLY+R4CH3=>CH4+HCHO+RC8H15Y    1.0E+0011  0.000  7300.0  ! ROH 1011
C9H18OLY+R8CH3OO=>CH3OOH+HCHO+RC8H15Y    1.0E+0012  0.000  14550.0  ! ROH
1012
C9H18OLY+R11C2H5=>C2H6+HCHO+RC8H15Y    1.5E+0000  3.500  4140.0  ! ROH
1013
C6H12OLY+R1H=>H2+HCHO+RC5H9Y    5.4E+0004  2.500  -1900.0  ! ROH 1014
C6H12OLY+R2OH=>H2O+HCHO+RC5H9Y    3.0E+0006  2.000  -1520.0  ! ROH 1015
C6H12OLY+R3OOH=>H2O2+HCHO+RC5H9Y    6.4E+0003  2.600  12400.0  ! ROH 1016
C6H12OLY+R4CH3=>CH4+HCHO+RC5H9Y    1.0E+0011  0.000  7300.0  ! ROH 1017
C6H12OLY+R8CH3OO=>CH3OOH+HCHO+RC5H9Y    1.0E+0012  0.000  14550.0  ! ROH
1018
C6H12OLY+R11C2H5=>C2H6+HCHO+RC5H9Y    1.5E+0000  3.500  4140.0  ! ROH
1019

! Additions on dienes
C4H6Z2+R2OH=>RC3H5Y+HCHO    1.4E+0012  0.000  -1040.0  ! AD 1020!!!!!!ds
мйса toluиne
!
!C4H6Z2+R2OH=>RC3H5Y+HCHO    3.0E+0012  0.000  -1040.0  !
!
C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V    1.0E+0005  2.500  -1900.0  ! AD 1021
C6H10Y2+R2OH=>H2O+C4H6Z2+R10C2H3V    6.0E+0006  2.000  -1520.0  ! AD 1022
C6H10Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V    1.2E+0004  2.600  12400.0  ! AD
1023
C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD 1024
C6H10Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD
1025
C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V    3.0E+0000  3.500  4140.0  ! AD
1026
C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y    1.0E+0005  2.500  -1900.0  ! AD 1027
C7H12Y2+R2OH=>H2O+C4H6Z2+RC3H5Y    6.0E+0006  2.000  -1520.0  ! AD 1028
C7H12Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y    1.2E+0004  2.600  12400.0  ! AD 1029
C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD 1030
C7H12Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD
1031
C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y    3.0E+0000  3.500  4140.0  ! AD
1032
!C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1033
!C10H18Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+2C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1034
!C10H18Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z    1.2E+0004  2.600  12400.0
! AD 1035
!C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1036
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!C10H18Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1037
!C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1038
!C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1039
!C11H20Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+2C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1040
!C11H20Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1041
!C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1042
!C11H20Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1043
!C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z    3.0E+0000  3.500  4140.0
! AD 1044
!C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1045
!C8H14Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1046
!C8H14Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1047
!C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1048
!C8H14Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1049
!C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z    3.0E+0000  3.500  4140.0
! AD 1050
!C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1051
!C12H22Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+3C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1052
!C12H22Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+3C2H4Z    1.2E+0004  2.600  12400.0
! AD 1053
!C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1054
!C12H22Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1055
!C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1056
!C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1057
!C9H16Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+C2H4Z    6.0E+0006  2.000  -1520.0  ! AD
1058
!C9H16Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+C2H4Z    1.2E+0004  2.600  12400.0  !
AD 1059
!C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0  ! AD
1060
!C9H16Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0
! AD 1061
!C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z    3.0E+0000  3.500  4140.0  !
AD 1062
!C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1063
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!C14H26Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+4C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1064
!C14H26Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+4C2H4Z    1.2E+0004  2.600  12400.0
! AD 1065
!C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1066
!C14H26Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1067
!C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1068
!C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1069
!C15H28Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+4C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1070
!C15H28Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+4C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1071
!C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1072
!C15H28Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1073
!C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z    3.0E+0000  3.500  4140.0
! AD 1074
!C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1075
!C16H30Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+5C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1076
!C16H30Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+5C2H4Z    1.2E+0004  2.600  12400.0
! AD 1077
!C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1078
!C16H30Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1079
!C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1080
!C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1081
!C13H24Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+3C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1082
!C13H24Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+3C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1083
!C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1084
!C13H24Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1085
!C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z    3.0E+0000  3.500  4140.0
! AD 1086

! Diels Alder

! .Y termination
RC3H5Y+R1H=>C3H6Y    1.0E+0014  0.000  0.0  ! TER
1087 !!!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC3H5Y+R2OH=>C3H6OLY    1.0E+0013  0.000  0.0  ! TER 1088
RC3H5Y+R3OOH=>C3H6O2PY    5.0E+0012  0.000  0.0  ! TER 1089
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RC3H5Y+R4CH3=>C4H8Y    1.0E+0013  0.000  0.0  ! TER 1090
RC3H5Y+R5CHO=>C4H6OAY    1.0E+0013  0.000  0.0  ! TER 1091
RC3H5Y+R6CH2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1092
RC3H5Y+R8CH3OO=>HCHO+R7CH3O+R10C2H3V    1.0E+0013  0.000  0.0  ! TER 1093
RC3H5Y+R11C2H5=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1094
RC4H7Y+R1H=>C4H8Y    1.0E+0014  0.000  0.0  ! TER
1095!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC4H7Y+R2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1096
RC4H7Y+R3OOH=>C4H8O2PY    5.0E+0012  0.000  0.0  ! TER 1097
RC4H7Y+R4CH3=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1098
RC4H7Y+R5CHO=>C5H8OAY    1.0E+0013  0.000  0.0  ! TER 1099
RC4H7Y+R6CH2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1100
RC4H7Y+R8CH3OO=>HCHO+R7CH3O+RC3H5Y    1.0E+0013  0.000  0.0  ! TER 1101
RC4H7Y+R11C2H5=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1102
RC7H13Y+R1H=>C7H14Y    1.0E+0014  0.000  0.0  ! TER
1103!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC7H13Y+R2OH=>C7H14OLY    1.0E+0013  0.000  0.0  ! TER 1104
RC7H13Y+R3OOH=>C7H14O2PY    5.0E+0012  0.000  0.0  ! TER 1105
RC7H13Y+R4CH3=>C8H16Y    1.0E+0013  0.000  0.0  ! TER 1106
RC7H13Y+R5CHO=>C8H14OAY    1.0E+0013  0.000  0.0  ! TER 1107
RC7H13Y+R6CH2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1108
RC7H13Y+R8CH3OO=>HCHO+R7CH3O+RC6H11Y    1.0E+0013  0.000  0.0  ! TER 1109
RC7H13Y+R11C2H5=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1110
RC8H15Y+R1H=>C8H16Y    1.0E+0014  0.000  0.0  ! TER
1111!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC8H15Y+R2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1112
RC8H15Y+R3OOH=>C8H16O2PY    5.0E+0012  0.000  0.0  ! TER 1113
RC8H15Y+R4CH3=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1114
RC8H15Y+R5CHO=>C9H16OAY    1.0E+0013  0.000  0.0  ! TER 1115
RC8H15Y+R6CH2OH=>C9H18OLY    1.0E+0013  0.000  0.0  ! TER 1116
RC8H15Y+R8CH3OO=>HCHO+R7CH3O+RC7H13Y    1.0E+0013  0.000  0.0  ! TER 1117
RC8H15Y+R11C2H5=>C10H20Z    1.0E+0013  0.000  0.0  ! TER 1118
RC5H9Y+R1H=>C5H10Y    1.0E+0014  0.000  0.0  ! TER
1119!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC5H9Y+R2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1120
RC5H9Y+R3OOH=>C5H10O2PY    5.0E+0012  0.000  0.0  ! TER 1121
RC5H9Y+R4CH3=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1122
RC5H9Y+R5CHO=>C6H10OAY    1.0E+0013  0.000  0.0  ! TER 1123
RC5H9Y+R6CH2OH=>C6H12OLY    1.0E+0013  0.000  0.0  ! TER 1124
RC5H9Y+R8CH3OO=>HCHO+R7CH3O+RC4H7Y    1.0E+0013  0.000  0.0  ! TER 1125
RC5H9Y+R11C2H5=>C7H14Y    1.0E+0013  0.000  0.0  ! TER 1126
RC3H5Y+RC3H5Y=>C6H10Y2    1.0E+0013  0.000  0.0  ! TER 1127
RC3H5Y+RC4H7Y=>C7H12Y2    1.0E+0013  0.000  0.0  ! TER 1128
RC3H5Y+RC7H13Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1129
RC3H5Y+RC8H15Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1130
RC3H5Y+RC5H9Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1131
RC4H7Y+RC4H7Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1132
RC4H7Y+RC7H13Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1133
RC4H7Y+RC8H15Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1134
RC4H7Y+RC5H9Y=>C9H16Y2    1.0E+0013  0.000  0.0  ! TER 1135
!RC7H13Y+RC7H13Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1136
!RC7H13Y+RC8H15Y=>C15H28Y2    1.0E+0013  0.000  0.0  ! TER 1137
RC7H13Y+RC5H9Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1138
!RC8H15Y+RC8H15Y=>C16H30Y2    1.0E+0013  0.000  0.0  ! TER 1139
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RC8H15Y+RC5H9Y=>C13H24Y2    1.0E+0013  0.000  0.0  ! TER 1140
!RC8H15Y+RC6H11Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1141
RC5H9Y+RC5H9Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1142
RC5H9Y+RC6H11Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1143

!
**********************************************************************
**!
!especes excitees!
R1H+B1O+M=OHE+M                   6.0E14      0.0      6.94E3     !
<HALL05>!
B4CH+O2=B2CO+OHE                  4.0E13      0.0      0.0        !
<HALL05>!
OHE+AR=R2OH+AR                    5.2E10      0.5      0.0        !
<HALL05>!
OHE+H2O=R2OH+H2O                  8.6E12      0.5      0.0        !
<HALL05>!
OHE+H2=R2OH+H2                    1.5E12      0.5      0.0        !
<HALL05>!
OHE+R1H=R2OH+R1H                  1.5E12      0.5      0.0        !
<HALL05>!
OHE+O2=R2OH+O2                    1.5E12      0.5      0.0        !
<HALL05>!
OHE+B1O=R2OH+B1O                  1.5E12      0.5      0.0        !
<HALL05>!
OHE+R2OH=R2OH+R2OH                1.5E12      0.5      0.0        !
<HALL05>!
OHE=>R2OH                            1.4E6       0.0      0.0        !
<HALL05>!
OHE+CO2=R2OH+CO2                  2.75E12     0.5     -968.      !
<HALL05>!
OHE+B2CO=R2OH+B2CO                3.23E12     0.5     -787.      !
<HALL05>!
OHE+CH4=R2OH+CH4                  3.36E12     0.5     -635.      !
<HALL05>!
R9C2H+B1O=B2CO+CHE                6.2E12      0.0      0.0        !
<HALL05>!
R9C2H+O2=CO2+CHE                  2.17E10     0.0      0.0        !
<HALL05>!
CHE+AR=B4CH+AR                    4.0E10      0.5      0.0        !
<HALL05>!
CHE+O2=B4CH+O2                    2.48E6      2.14     0.0        !
<HALL05>!
CHE+H2O=B4CH+H2O                  5.3E13      0.0      0.0        !
<HALL05>!
CHE+H2=B4CH+H2                    1.47E14     0.0      1360.      !
<HALL05>!
CHE+CO2=B4CH+CO2                  2.41E-1     4.3     -1694.          !
<HALL05>!
CHE+B2CO=B4CH+B2CO                2.44E12     0.5      0.0       !
<HALL05>!
CHE+CH4=B4CH+CH4                  1.73E13     0.0      167.      !
<HALL05>!
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CHE=>B4CH                              1.86E6      0.0      0.0        !
<HALL05>!


!*****************************************!
!     REACTIONS DE LA MATRICE O(0)C(y)H(z)   !
!*****************************************!

!****** REACTIONS DE H2******!
R1H+R1H+M=H2+M                 1.87E18     -1.00     0.00
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/
AR/0.35/
!      N2/0.4/ HE/0.35/

!****** REACTIONS DE B4CH ******!
B4CH+R1H=B3C+H2              7.8E13       0.       0.       !(2,-
2)<PEETERS97>!

!****** REACTIONS DE B6CH2 ******!
B6CH2+M=B5CH2+M                1.51E13      0.0      0.0
       O2/.4/ B2CO/.75/ CO2/1.5/ H2O/6.5/ CH4/.48/  C2H4Z/1.6/
      AR/.24/
B6CH2+R1H=B4CH+H2              3.0E13       0.       0.           !(4,-
4)<TSAnG86>!

!****** REACTIONS DE B5CH2 ******!
B5CH2+R1H=B4CH+H2              6.0E12       0.      -1.8E3        !(5,-
5)<BAULCH94>!
B5CH2+B3C=R9C2H+R1H           5.0E13       0.       0.           !(6,-
6)<RAnZI94>!
B5CH2+B5CH2=>C2H2+R1H+R1H      1.2E14       0.       0.8E3        !
(7)<BAULCH94>!

!****** REACTIONS DE R4CH3 ******!
R4CH3+M=B5CH2+R1H+M                2.91E16     0.0     90.7E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R4CH3+R1H=B6CH2+H2              6.0E13      0.        15.0E3           !
(9,-9)<BAULCH94>!
R4CH3+B4CH=R10C2H3V+R1H         3.0E13      0.         0.          !(10,-
10)<DAGAUT91>
R4CH3+B6CH2=C2H4Z+R1H           1.8E13      0.         0.          !(11,-
11)<TSAnG86>!
R4CH3+B5CH2=C2H4Z+R1H           4.2E13      0.         0.          !(12,-
12)<BAULCH94>!
R4CH3+B3C=C2H2+R1H             5.0E13      0.         0.           !(13,-
13)<RAnZI94>!
R4CH3+R4CH3(+M)=>C2H6(+M)       3.61E13     0.         0.          !
(14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.63E41  -7.0   2.76E3 /
      TROE /  0.62  73  1180 /
```

```
C2H6(+M)=>R4CH3+R4CH3(+M)     1.8E21      -1.24    90.9E3        !(-
14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 1.89E49   -8.24   93.7E3/
      TROE /  0.62  73  1180 /
R4CH3+R4CH3=R11C2H5+R1H        3.0E13      0.      13.5E3        !(15,-
15)<BAULCH94>!
R4CH3+R4CH3=C2H4Z+H2           2.1E14      0.      19.3E3        !(16,-
16)<FRAnK86nIST>!

!****** REACTIONS DE CH4 ******!
R1H+R4CH3(+M)=>CH4(+M)         1.67E14     0.      0.            !
(17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW /  1.408E24  -1.8   0.0 /
      TROE / 0.37 3315 61 /
CH4(+M)=>R4CH3+R1H(+M)         2.4E16      0.    105.0E3         !(-
17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/
!     N2/0.4/ HE/0.35/
      LOW / 1.29E18    0.00  90.9E3 /
      TROE / 0  1350  1  7830 /
CH4(+CH4)=>R4CH3+R1H(+CH4)     2.4E16      0.    105.0E3         !(-
17')<BAULCH94>!
      LOW / 8.43E17    0.00  90.9E3 /
      TROE / 0.69  90  2210 /
CH4+R1H=R4CH3+H2               1.3E04      3.      8.0E3         !(18,-
18)<BAULCH94>!
CH4+B4CH=C2H4Z+R1H             3.0E13      0.     -0.4E3         !(19,-
19)<DAGAUT91BAULCH94>!
CH4+B6CH2=R4CH3+R4CH3          4.2E13      0.      0.            !(20,-
20)<TSAnG86>!

!****** REACTIONS DE R9C2H ******!
R9C2H+B6CH2=C2H2+B4CH          1.8E13      0.         0.         !(21,-
21)<TSAnG86>!
R9C2H+B5CH2=C2H2+B4CH          1.8E13      0.         0.         !(22,-
22)<TSAnG86>!
R9C2H+CH4=C2H2+R4CH3           1.2E12      0.         0.         !(23,-
23)<BAULCH94>!

!****** REACTIONS DE C2H2 ******!
C2H2+M=R9C2H+R1H+M             1.14E17     0.    107.0E3         !(24,-
24)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H2+R1H=R9C2H+H2              6.6E13      0.     27.7E3         !(25,-
25)<BAULCH94>!

!****** REACTIONS DE R10C2H3V ******!
R10C2H3V(+M)=C2H2+R1H(+M)      2.0E14      0.     39.8E3         !(26,-
26)<BAULCH94>!
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      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 1.19E42  -7.50  45.55E3 /
      TROE    /0.35   1.0       1.E8/
R10C2H3V+R1H=C2H2+H2          1.2E13      0.         0.          !(27,-
27)<BAULCH94>!
R10C2H3V+B6CH2=C2H2+R4CH3     1.8E13      0.         0.          !(28,-
28)<TSAnG86>!
R10C2H3V+B5CH2=C2H2+R4CH3     1.8E13      0.         0.          !(29,-
29)<TSAnG86>!
R10C2H3V+R4CH3=CH4+C2H2       3.9E11      0.         0.          !(30,-
30)<TSAnG86>!
R10C2H3V+R9C2H=2C2H2          9.6E11      0.         0.          !(31,-
31)<TSAnG86>!
R10C2H3V+R10C2H3V=C2H4Z+C2H2  9.6E11      0.         0.          !(32,-
32)<TSAnG86>!

!****** REACTIONS DE C2H4Z ******!
C2H4Z+M=C2H2+H2+M             9.97E16     0.     71.6E3          !(33,-
33)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H4Z+M=R10C2H3V+R1H+M        7.40E17     0.     96.7E3          !(34,-
34)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!C2H4Z+R1H=R10C2H3V+H2        5.4E14      0.     14.8E3          !(35,-
35)<BAULCH94>!
C2H4Z+R1H=R10C2H3V+H2         5.0E7       1.93   13.0E3          !(35,-
35)SLAGLE96!
!C2H4Z+R4CH3=CH4+R10C2H3V     4.1E12      0.     11.1E3          !(36,-
36)<BAULCH94>!
C2H4Z+R4CH3=CH4+R10C2H3V      6.3E11      0.     16.0E3          !(36,-
36)BACK89!

!****** REACTIONS DE R11C2H5 ******!
!C2H4Z+R1H(+M)=>R11C2H5(+M)    3.97E09    1.28     1.3E3
!      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!      LOW / 1.35E19   0.00   0.76E3 /
!      TROE / 0.76  40  1025/
R11C2H5(+M)=C2H4Z+R1H(+M)      8.2E13      0.    40.0E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.40E17   0.00   33.4E3 /
      TROE / 0.75  97  1379/
R11C2H5+R1H=C2H4Z+H2           1.8E12      0.         0.          !(38,-
38)<TSAnG86>!
R11C2H5+R1H=C2H6               3.6E13      0.         0.          !(39,-
39><TSAnG86>!
R11C2H5+B6CH2=C2H4Z+R4CH3      9.0E12      0.         0.          !(40,-
40)<TSAnG86>!
R11C2H5+B5CH2=C2H4Z+R4CH3      1.8E13      0.         0.          !(41,-
41)<TSAnG86>!
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R11C2H5+R4CH3=C2H4Z+CH4        1.1E12      0.          0.         !(42,-
42)<BAULCH94>!
R11C2H5+R9C2H=C2H2+C2H4Z       1.8E12      0           0.         !(43,-
43)<TSAnG86>!
R11C2H5+R10C2H3V=2C2H4Z        4.8E11      0.          0.         !(44,-
44)<TSAnG86>!
R11C2H5+R10C2H3V=C2H2+C2H6     4.8E11      0.          0.         !(45,-
45)<TSAnG86>!
R11C2H5+R11C2H5=C2H4Z+C2H6     1.4E12      0.          0.         !(46,-
46)<BAULCH94>!

!****** REACTIONS DE C2H6 ******!
C2H6+M=C2H4Z+H2+M              2.3E17      0.     67.4E3          !(47,-
47)<SCHULTZ85nIST>!
C2H6+R1H=R11C2H5+H2            1.4E9       1.5     7.4E3          !(48,-
48)<BAULCH94>!
C2H6+B6CH2=R4CH3+R11C2H5       1.1E14      0.          0.         !(49,-
49)<TSAnG86>!
C2H6+R4CH3=R11C2H5+CH4         1.5E-7      6.0     5.8E3          !(50,-
50)<BAULCH94>!
C2H6+R9C2H=C2H2+R11C2H5        3.6E12      0.          0.         !(51,-
51)<TSAnG86>!
C2H6+R10C2H3V=R11C2H5+C2H4Z    6.0E2       3.3    10.5E3          !(52,-
52)<TSAnG86>!


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!*****************************************************!
!          REACTIONS DE LA MATRICE O(x)C(y)H(z)  x>0      !
!*****************************************************!

!****** REACTIONS DE B1O ******!
B1O+H2=R2OH+R1H                5.1E4       2.67    6.2E3          !(53,-
53)<BAULCH94>!
B1O+B4CH=B2CO+R1H              3.9E13      0.          0.         !(54,-
54)<BAULCH94>!
B1O+B4CH=B3C+R2OH             1.5E13      0.     4.7E3           !(55,-
55)<MUR86nIS>!
B1O+B6CH2=>B2CO+2R1H           1.5E13      0.          0.         !(56)
<TSAnG86>!
B1O+B6CH2=B2CO+H2              1.5E13      0.          0.         !(57,-57)
<TSAnG86>!
B1O+B5CH2=>B2CO+2R1H           7.2E13      0.          0.         !(58)
<BAULCH94>!
B1O+B5CH2=B2CO+H2              4.8E13      0.          0.         !(59,-
59)<BAULCH94>!
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B1O+R4CH3=HCHO+R1H              8.4E13      0.          0.         !(60,-
60)<BAULCH94>!
B1O+R4CH3=R7CH3O                8.0E15     -2.12     0.6E3         !(61,-
61)<DEAn87nIS>!
B1O+CH4=R4CH3+R2OH              7.2E8       1.56     8.4E3         !(62,-
62)<BAULCH94>!
B1O+R9C2H=B4CH+B2CO             1.0E13      0.          0.         !(63,-
63)<DAGAUT91>!
B1O+C2H2=B5CH2+B2CO             2.17E06     2.1      1.6E3         !(64,-
64)<BAULCH LEEDS>!
B1O+C2H2=R12CHCOZ+R1H           5.06E06     2.1      1.6E3         !(65,-
65)<BAULCH LEEDS>!
R2OH+R9C2H=C2H2+B1O             1.8E13      0.          0.        !(89,-
89)<TSANG86>! modif MF
B1O+R10C2H3V=R4CH3+B2CO         3.0E13      0.          0.         !(66,-
66)<DAGAUT91>!
B1O+R10C2H3V=CH2COZ+R1H         9.6E13      0.          0.         !(67,-
67)<TSAnG86>!
B1O+C2H4Z=R4CH3+R5CHO           8.1E6       1.88     0.2E3         !(68,-
68)<BAULCH94>!
B1O+C2H4Z=HCHO+B5CH2            4.00E5      1.88     0.2E3         !(69,-
69)<BAULCH94>!
B1O+C2H4Z=CH2COZ+H2             6.6E5       1.88     0.2E3         !(70,-
70)<BAULCH94>!
B1O+C2H4Z=R13CH2CHO+R1H         4.7E6       1.88     0.2E3         !(71,-
71)<BAULCH94>!
B1O+C2H4Z=R2OH+R10C2H3V         1.5E7       1.91     3.7E3         !(72,-
72)<MAHMUD87nIST>!
B1O+R11C2H5=HCHO+R4CH3          1.1E13      0.          0.         !(73,-
73)<BAULCH94>!
B1O+R11C2H5=CH3CHO+R1H          5.5e13      0.          0.         !(74,-
74)<BAULCH94>!
B1O+R11C2H5=C2H4Z+R2OH          3.0E13      0.          0.         !(75,-
75)<DAGAUT91>!
B1O+C2H6=R11C2H5+R2OH           1.0E9       1.5      5.8E3         !(76,-
76)<BAULCH94>!

!****** REACTIONS DE R2OH ******!
R1H+B1O+M=R2OH+M                1.18E19    -1.0       0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R1H+R2OH+M=H2O+M                 5.53E+22   -2.0         0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/
!      N2/0.4/ HE/0.35/
R2OH+H2=R1H+H2O                 1.0E8       1.6      3.3E3         !(79,-
79)<BAULCH94>!
R2OH+B3C=B2CO+R1H              5.0E13      0.          0.         !(80,-
80)<RAnZI94>!
R2OH+B4CH=R5CHO+R1H             3.0E13      0.          0.         !(81,-
81)<DAGAUT91>!
R2OH+B6CH2=HCHO+R1H             3.0E13      0.          0.         !(82,-
82)<TSAnG86>!
R2OH+B5CH2=HCHO+R1H             1.8E13      0.          0.         !(83,-
83)<TSAnG86>!
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R2OH+R4CH3=B6CH2+H2O           7.2E13      0.      2.7E3        !(84,-
84)<BAULCH94>!
R2OH+R4CH3(+M)=CH3OH(+M)       6.0E13      0.         0.        !(85,-
85)<BAULCH94>!
      LOW     /1.4E44     -8.2          0./
      TROE    /0.82      200.        1438./
R2OH+R4CH3=HCHO+H2             3.2E12     -0.53   10.8E3       !(86,-
86)<DAGAUT91>!
R2OH+R4CH3=R7CH3O+R1H          5.7E12     -0.23   13.9E3       !(87,-
87)<DAGAUT91>!
R2OH+CH4=R4CH3+H2O             1.6E7       1.83    2.7E3       !(88,-
88)<BAULCH94>!
!R2OH+R9C2H=C2H2+B1O           1.8E13      0.         0.        !(89,-
89)<TSAnG86>!
R2OH+R9C2H=B5CH2+B2CO          1.8E13      0.         0.        !(90,-
90)<TSAnG86>!
R2OH+R9C2H=R12CHCOZ+R1H        2.0E13      0.         0.        !(91,-
91)<DAGAUT91>!
R2OH+C2H2=R9C2H+H2O            3.385E+07   2.0   14000.0       !(92,-
92)<KONNOV00>!
R2OH+C2H2=CH2COZ+R1H           1.100E+13   0.0    7170.0       !(93,-
93)<KONNOV00>!
R2OH+C2H2=R4CH3+B2CO           4.8E-4      4.     -2.0E3       !(94,-
94)<DAGAUT91>!
R2OH+R10C2H3V=C2H2+H2O         3.0E13      0.         0.        !(95,-
95)<TSAnG86>!
R2OH+R10C2H3V=CH3CHO           3.0E13      0.         0.        !(96,-
96)<TSAnG86>!
R2OH+C2H4Z=R10C2H3V+H2O        2.0E13      0.      5.9E3        !(97,-
97)<BAULCH94>!
R2OH+C2H4Z=R4CH3+HCHO          2.0E12      0.      0.9E3        !(98,-
98)<GLARBORG86>!
R2OH+R11C2H5=C2H4Z+H2O         2.4E13      0.         0.        !(99,-
99)<TSAnG86>!
R2OH+R11C2H5=>R4CH3+R1H+HCHO   2.4E13      0.         0.        !(100)
<TSAnG86>!
R2OH+C2H6=R11C2H5+H2O          7.2E6       2.      0.9E3        !(101,-
101)<BAULCH94>!
R2OH+R2OH=H2O+B1O              1.5E9       1.14    0.1E3        !(102,-
102)<BAULCH94>!

!****** REACTIONS DE H2O ******!
H2O+B4CH=R6CH2OH               5.7E12      0.     -0.8E3        !(103,-
103)<BAULCH94>!
H2O+B6CH2=CH3OH                1.8E13      0.         0.        !(104,-
104)<TSAnG86>!

!REACTIOnS DE B2CO!
B2CO+R4CH3(+M)=R14CH3CO(+M)    5.0E11      0.      6.9E3        !(105,-
105)<BAULCH94>!
       LOW    /1.1E14      0.      3.8E3/
       TROE   /0.5         1.0      1.0E8/
B2CO+B1O+M=CO2+M               1.54E15     0.0     3.0E3        !(106,-
106)<TSAnG86>!
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       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
B2CO+R2OH=CO2+R1H              6.3E6       1.5    -0.5E3        !(107,-
107)<BAULCH94>!

!REACTIOnS DE R5CHO!
R5CHO+M=R1H+B2CO+M             1.9E17     -1.     17.0E3        !(108,-
108)<WAnG97>!
       H2/2.0/ B2CO/1.5/ CO2/2.0/ H2O/6.0/
R5CHO+R1H=H2+B2CO              9.0E13      0.         0.        !(109,-
109)<BAULCH94>!
R5CHO+R1H=B1O+B5CH2            4.0E13      0.    102.5E3        !(110,-
110)<TSUBOI81nIST>!
R5CHO+B6CH2=R4CH3+B2CO         1.8E13      0.         0.        !(111,-
111)<TSAnG86>!
R5CHO+B5CH2=R4CH3+B2CO         1.8E13      0.         0.        !(112,-
112)<TSAnG86>!
R5CHO+R4CH3=CH4+B2CO           1.2E14      0.         0.        !(113,-
113)<TSAnG86>!
R5CHO+R4CH3=CH3CHO             1.8E13      0.         0.        !(114,-
114)<TSAnG86>!
R4CH3+HCHO=R5CHO+CH4           7.7E-8      6.1    1.97E3        !(115,-
115)<BAULCH94>!
R5CHO+R9C2H=C2H2+B2CO          6.0E13      0.         0.        !(116,-
116)<TSAnG86>!
R5CHO+R10C2H3V=C2H4Z+B2CO      9.0E13      0.         0.        !(117,-
117)<TSAnG86>!
R10C2H3V+HCHO=R5CHO+C2H4Z      5.4E3       2.81    5.9E3        !(118,-
118)<TSAnG86>!
R5CHO+R11C2H5=C2H6+B2CO        1.2E14      0.         0.        !(119,-
119)<TSAnG86>!
R11C2H5+HCHO=R5CHO+C2H6        5.57E3      2.81   5.86E3        !(120,-
120)<TSAnG86>!
R5CHO+B1O=R1H+CO2              3.0E13      0.         0.        !(121,-
121)<BAULCH94>!
R5CHO+B1O=R2OH+B2CO            3.0E13      0.         0.        !(122,-
122)<BAULCH94>!
R5CHO+R2OH=H2O+B2CO            1.1E14      0.         0.        !(123,-
123)<BAULCH94>!
R5CHO+R5CHO=HCHO+B2CO          3.0E13      0.         0.        !(124,-
124)<BAULCH94>!

!****** REACTIONS DE HCHO ******!
HCHO+M=R5CHO+R1H+M             1.40E36    -5.54   96.8E3        !(125,-
125)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+M=H2+B2CO+M               3.26E36    -5.54   96.8E3        !(126,-
126)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+R1H=R5CHO+H2              1.3E8       1.62    2.1E3        !(127,-
127)<BAULCH94>!
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HCHO+B4CH=R13CH2CHO            9.6E13      0.     -0.5E3        !(128,-
128)<BAULCH94average>!
HCHO+B6CH2=R4CH3+R5CHO         1.2E12      0.         0.        !(129,-
129)<TSAnG86>!
HCHO+B1O=R5CHO+R2OH            4.1E11      0.57    2.7E3        !(130,-
130)<BAULCH94>!
HCHO+R2OH=R5CHO+H2O            7.82E07     1.63  -1.06E3        !MF
Vasudevan Int. J. Chem. Kin. 37(2005)98–109

!****** REACTIONS DE R7CH3O ******!
R7CH3O+M=HCHO+R1H+M             1.55E14     0.00   13.5E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R7CH3O+R1H=HCHO+H2             1.8E13      0.         0.        !(133,-
133)<BAULCH94>!
R7CH3O+B6CH2=R4CH3+HCHO        1.8E13      0.         0.        !(134,-
134)<TSAnG86>!
R7CH3O+B5CH2=R4CH3+HCHO        1.8E13      0.         0.        !(135,-
135)<TSAnG86>!
R7CH3O+R4CH3=HCHO+CH4          2.4E13      0.         0.        !(136,-
136)<TSAnG86>!
R7CH3O+CH4=R4CH3+CH3OH         1.6E11      0.      8.8E3        !(137,-
137)<TSAnG86>!
R7CH3O+R9C2H=HCHO+C2H2         2.4E13      0.         0.        !(138,-
138)<TSAnG86>!
R7CH3O+R10C2H3V=HCHO+C2H4Z     2.4E13      0.         0.        !(139,-
139)<TSAnG86>!
R7CH3O+C2H4Z=HCHO+R11C2H5      1.2E11      0.      6.7E3        !(140,-
140)<TSAnG86>!
R7CH3O+R11C2H5=HCHO+C2H6       2.4E13      0.         0.        !(141,-
141)<TSAnG86>!
R7CH3O+C2H6=R11C2H5+CH3OH      2.4E11      0.      7.0E3        !(142,-
142)<TSAnG86>!
R7CH3O+B1O=HCHO+R2OH           1.8E12      0.         0.        !(143,-
143)<BAULCH94>!
R7CH3O+R2OH=HCHO+H2O           1.8E13      0.         0.        !(144,-
144)<TSAnG86>!
R7CH3O+B2CO=R4CH3+CO2          1.6E13      0.     11.7E3        !(145,-
145)<TSAnG86>!
R7CH3O+R5CHO=CH3OH+B2CO        9.1E13      0.         0.        !(146,-
146)<TSAnG86>!
R7CH3O+HCHO=CH3OH+R5CHO        1.0E11      0.      3.0E3        !(147,-
147)<TSAnG86>!
R7CH3O+R7CH3O=CH3OH+HCHO       6.0E13      0.         0.        !(148,-
148)<TSAnG86>!


!****** REACTIONS DE R6CH2OH ******!
R6CH2OH+M=HCHO+R1H+M           1.26E16     0.00   30.0E3        !(149,-
149)<BAULCHLEEDS>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R6CH2OH+R1H=R4CH3+R2OH         9.6E13      0.         0.        !(150,-
150)<TSAnG87>!
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R6CH2OH+R1H=HCHO+H2            6.0E12      0.          0.         !(151,-
151)<TSAnG87>!
R6CH2OH+H2=CH3OH+R1H           6.7E5       2.      13.4E3         !(152,-
152)<TSAnG87>!
R6CH2OH+B6CH2=CH3CHO+R1H       1.8E13      0.          0.         !(153,-
153)<TSAnG87>!
R6CH2OH+B5CH2=C2H4Z+R2OH       2.4E13      0.          0.         !(154,-
154)<TSAnG87>!
R6CH2OH+B5CH2=R4CH3+HCHO       1.2E12      0.          0.         !(155,-
155)<TSAnG87>!
R6CH2OH+R4CH3=C2H5OH          1.2E13      0.          0.         !(156,-
156)<TSAnG87>!
R6CH2OH+R4CH3=CH4+HCHO         2.4E12      0.          0.         !(157,-
157)<TSAnG87>!
R6CH2OH+CH4=CH3OH+R4CH3        21.7        3.1    16.2E3         !(158,-
158)<TSAnG87>!
R6CH2OH+R9C2H=C2H2+HCHO        4.8E13      0.          0.         !(159,-
159)<TSAnG87>!
!la constante de vitesse du processus 159 est globalisee!
!R6CH2OH+R9C2H=C3H3+R2OH       1.2E13      0.          0.         !(159a,-
159a)<TSAnG87>!
!R6CH2OH+R9C2H=C2H2+HCHO       3.6E13      0.          0.         !(159b,-
159b)<TSAnG87>!
R6CH2OH+C2H2=R10C2H3V+HCHO     7.2E11      0.      9.0E3          !(160,-
160)<TSAnG87>!
R6CH2OH+R10C2H3V=C2H4Z+HCHO    4.2E13      0.          0.         !(161,-
161)<TSAnG87>!
!La constante de vitesse  du processus 161 est globalisee!
R6CH2OH+R11C2H5=C2H4Z+CH3OH    2.4E12      0.          0.         !(162,-
162)<TSAnG87>!
R6CH2OH+R11C2H5=C2H6+HCHO      2.4E12      0.          0.         !(163,-
163)<TSAnG87>!
R6CH2OH+C2H6=CH3OH+R11C2H5     199.        3.      14.0E3         !(164,-
164)<TSAnG87>!
R6CH2OH+B1O=HCHO+R2OH          4.2E13      0.          0.         !(165,-
165)<TSAnG87>!
R6CH2OH+R2OH=H2O+HCHO          2.4E13      0.          0.         !(166,-
166)<TSAnG87>!
!attention (167) metatheses dans les reactions de CH3OH!
!R6CH2OH+H2O=CH3OH+R2OH        1.6E14      0.      26.3E3         !(167,-
167)<TSUBOI81nIST>!
R6CH2OH+R5CHO=CH3OH+B2CO       1.2E14      0.          0.         !(168,-
168)<TSAnG87>!
R6CH2OH+R5CHO=HCHO+HCHO        1.8E14      0.          0.         !(169,-
169)<TSAnG87>!
R6CH2OH+HCHO=CH3OH+R5CHO       5.5E3       2.8      5.9E3         !(170,-
170)<TSAnG87>!
R6CH2OH+R7CH3O=CH3OH+HCHO      2.4E13      0.          0.         !(171,-
171)<TSAnG87>!
R6CH2OH+R6CH2OH=CH3OH+HCHO     1.4E13      0.          0.         !(172,-
172)<TSAnG87>!
!la constante de vitesse du processus 172 est globalisee!
!R6CH2OH+R6CH2OH=CH3OH+HCHO    4.8E12      0.          0.         !(172a,-
172a)<TSAnG87>!
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!R6CH2OH+R6CH2OH=HOCH2CH2OH    9.6E12      0.          0.         !(172b,-
172b)<TSAnG87>!

!****** REACTIONS DE CH3OH ******!
CH3OH+R1H=R4CH3+H2O            2.0E14      0.       5.3E3         !(173,-
173)<HIDAKA89nIST>!
CH3OH+R1H=R7CH3O+H2            4.2E6       2.1      4.9E3         !(174,-
174)<TSAnG87>!
CH3OH+B6CH2=R6CH2OH+R4CH3      1.5E12      0.          0.         !(175,-
175)<TSAnG87>!
CH3OH+B5CH2=R4CH3+R6CH2OH      31.9        3.2      7.2E3         !(176,-
176)<TSAnG87>!
CH3OH+B5CH2=R4CH3+R7CH3O       14.4        3.1      6.9E3         !(177,-
177)<TSAnG87>!
CH3OH+R9C2H=C2H2+R6CH2OH       6.0E12      0.          0.         !(178,-
178)<TSAnG87>!
CH3OH+R9C2H=C2H2+R7CH3O        1.2E12      0.          0.         !(179,-
179)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R6CH2OH   31.9        3.2      7.2E3         !(180,-
180)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R7CH3O    14.4        3.1      6.9E3         !(181,-
181)<TSAnG87>!
CH3OH+B1O=R6CH2OH+R2OH         3.4E13      0.       5.5E3          !(182,-
182)<GROTHEER81nIST>!
CH3OH+B1O=R7CH3O+R2OH          1.0E13      0.       4.7E3         !(183,-
183)<WARnATZ84>!
!modification des metatheses avec OH!
!CH3OH+R2OH=R7CH3O+H2O         1.0E13      0.       1.7E3         !(184,-
184)<WARnATZ84>!
CH3OH+R2OH=R6CH2OH+H2O         3.1E06      2.      -3.4E2         !(184a,-
184a)<Atkinson86>85%!
CH3OH+R2OH=R7CH3O+H2O          5.4E05      2.      -3.4E2         !(184b,-
184b)<Atkinson86>15%!
CH3OH+R7CH3O=CH3OH+R6CH2OH     3.0E11      0.       4.1E3         !(185,-
185)<TSAnG87>!

!****** REACTIONS DE R12CHCOD ******!
R12CHCOZ+M=B4CH+B2CO+M          6.0E15      0.      58.8E3         !(186,-
186)<DAGAUT91>!
R12CHCOZ+R1H=B5CH2+B2CO         1.5E14      0.          0.         !(187a,-
187a)<BAULCH94>!
R12CHCOZ+R1H=B6CH2+B2CO         1.3E14      0.          0.         !(187b,-
187b)<PEETERS97>!
R12CHCOZ+B5CH2=R9C2H+HCHO       1.0E13      0.       2.0E3         !(188,-
188)<DAGAUT91>!
R12CHCOZ+B5CH2=R10C2H3V+B2CO    3.0E13      0.          0.         !(189,-
189)<DAGAUT91>!
R12CHCOZ+B1O=>B2CO+B2CO+R1H     9.6E13      0.          0.         !
(190)<BAULCH94>!
R12CHCOZ+R2OH=>R5CHO+B2CO+R1H   1.0E13      0.          0.         !
(191)<DAGAUT91>!


!****** REACTIONS DE CH2COD ******!
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```
CH2COZ+M=B6CH2+B2CO+M          6.57E15     0.0    57.6E3        !(192,-
192)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
CH2COZ+M=R12CHCOZ+R1H+M        2.7E17      0.     87.0E3        !(193,-
193)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
CH2COZ+R1H=R4CH3+B2CO          1.8E13      0.      3.4E3        !(194,-
194)<BAULCH94>!
CH2COZ+R1H=R12CHCOZ+H2         5.0E13      0.      8.0E3        !(195,-
195)<DAGAUT91>!
CH2COZ+B5CH2=C2H4Z+B2CO        1.3E14      0.         0.        !(196,-
196)<CAnOSA-MAS84nIST>!
CH2COZ+B1O=B5CH2+CO2           1.8E12      0.      1.3E3        !(197,-
197)<DAGAUT91>!
CH2COZ+B1O=R12CHCOZ+R2OH       1.0E13      0.      8.0E3        !(198,-
198)<DAGAUT91>!
CH2COZ+R2OH=R12CHCOZ+H2O       7.5E12      0.      2.0E3        !(199,-
199)<DAGAUT91>!
!CH2COZ+R2OH=R5CHO+HCHO        2.8E13      0.        0.         !(200,-
200)<VAnDOOREn77nIST>!
CH2COZ+R2OH=R4CH3+CO2          2.52E12     0.         0.        !(200a,-
200a)<BAULCH LEEDS>!
CH2COZ+R2OH=R6CH2OH+B2CO       4.68E12     0.         0.        !(200b,-
200b)<BAULCH LEEDS>!


!****** REACTIONS DE R14CH3CO ******!
R14CH3CO+R1H=R4CH3+R5CHO        9.6E13      0.         0.        !(201,-
201)<TSAnG86>!
R14CH3CO+B6CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(202,-
202)<TSAnG86>!
R14CH3CO+B5CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(203,-
203)<TSAnG86>!
R14CH3CO+B1O=R4CH3+CO2          9.6E12      0.         0.        !(204,-
204)<TSAnG86>!
R14CH3CO+R2OH=CH2COZ+H2O        1.2E13      0.         0.        !(205,-
205)<TSAnG86>!
R14CH3CO+R2OH=>R4CH3+B2CO+R2OH  3.0E13      0.         0.        !
(206)<TSAnG86>!
R14CH3CO+R5CHO=CH3CHO+B2CO      9.0E12      0.         0.        !(207,-
207)<TSAnG86>!
R14CH3CO+HCHO=CH3CHO+R5CHO      1.8E11      0.     12.9E3        !(208,-
208)<TSAnG86>!
R14CH3CO+R7CH3O=CH3OH+CH2COZ    6.0E12      0.         0.        !(209,-
209)<TSAnG86>!
R14CH3CO+R7CH3O=HCHO+CH3CHO     6.0E12      0.         0.        !(210,-
210)<TSAnG86>!
R14CH3CO+CH3OH=CH3CHO+R6CH2OH   4.85E3      3.     12.3E3        !(211,-
211)<TSAnG87>!
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 1.2E13      0.         0.        !(212,-
212)<TSAnG86>!
```

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!****** REACTIONS DE R13CH2CHO ******!
!R13CH2CHO=R14CH3CO               1.0E13      0.      47.0E3          !
(213,-213)<COLKET75nIST>!
!R13CH2CHO=R1H+CH2COZ             1.6E13      0.      35.0E3          !
(214,-214)<COLKET75nIST>!
R13CH2CHO=R4CH3+B2CO                 2.93E12     0.29    40.3E3!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.
R13CH2CHO=R1H+CH2COZ                1.43E15     -0.15   45.6E3 !at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.


!****** REACTIONS DE CH3CHO ******!
!CH3CHO+R1H=H2+R14CH3CO           4.0E13      0.       4.2E3          !
(215,-215)<WARnATZ84>!
!CH3CHO+R4CH3=R14CH3CO+CH4        2.0E-6      5.6      2.5E3          !
(216,-216)<BAULCH94>!
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO   8.1E10      0.       3.7E3          !
(217,-217)<SCHERZER87>!
!CH3CHO+R11C2H5=C2H6+R14CH3CO     1.3E12      0.       8.5E3          !
(218,-218)<HOHLEIn70>!
!CH3CHO+B1O=R14CH3CO+R2OH         1.4E13      0.       2.3E3          !
(219,-219)<CAVAnAGH90>!
!CH3CHO+R2OH=R14CH3CO+H2O         4.2E12      0.       0.5E3          !
(220,-220)<CAVAnAGH90>!
!CH3CHO+R7CH3O=R14CH3CO+CH3OH     2.4E11      0.       1.8E3          !
(221,-221)<CAVAnAGH90>!
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 2.5E7       0.         0.           !
(222,-222)<SCHUCHMAnn70nIST>!

!****** REACTIONS DE C2H4O# ******!
C2H4O#3=CH4+B2CO                  1.2E13      0.      57.2E3   !(223,-
223)<LIFSHITZ83nIST>!
C2H4O#3=CH3CHO                    7.3E13      0.      57.2E3   !(224,-
224)<LIFSHITZ83nIST>!
C2H4O#3=R4CH3+R5CHO               3.6E13      0.      57.2E3   !(225,-
225)<LIFSHITZ83nIST>!
C2H4O#3+R1H=H2+R13CH2CHO          2.0E13      0.       8.3E3   !(226,-
226)<LIFSHITZ83nIST*>!
C2H4O#3+R1H=H2O+R10C2H3V          5.0E9       0.       5.0E3   !(227,-
227)<LIFSHITZ83nIST>!
C2H4O#3+R1H=C2H4Z+R2OH            9.5E10      0.       5.0E3   !(228,-
228)<LIFSHITZ83nIST>!
C2H4O#3+R4CH3=CH4+R13CH2CHO       1.1E12      0.      11.8E3   !(229,-
229)<BALDWIn84nIST*>!
C2H4O#3+R4CH3=R11C2H5+HCHO        1.4E11      0.       7.6E3   !(230,-
230)<RAnZI94>!
C2H4O#3+R4CH3=C2H4Z+R7CH3O        1.5E10      0.       7.6E3   !(231,-
231)<RAnZI94>!
C2H4O#3+R9C2H=C2H2+R13CH2CHO      1.2E12      0.       9.8E3   !(232,-
232)<RAnZI94>!
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO  2.0E12      0.       9.3E3   !(233,-
233)<RAnZI94>!
C2H4O#3+R11C2H5=C2H6+R13CH2CHO    6.8E11      0.      11.4E3   !(234,-
234)<RAnZI94>!
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C2H4O#3+B1O=R2OH+R13CH2CHO          1.9E12      0.       5.2E3    !(235,-
235)<BOGAn78nIST>!
C2H4O#3+R2OH=H2O+R13CH2CHO          1.8E13      0.       3.6E3    !(236,-
236)<BALDWIn84nIST*>!
C2H4O#3+R5CHO=HCHO+R13CH2CHO        3.7E12      0.      15.8E3    !(237,-
237)<RAnZI94>!
C2H4O#3+R7CH3O=CH3OH+R13CH2CHO      1.3E12      0.       5.8E3    !(238,-
238)<RAnZI94>!
C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO     8.4E11      0.      13.4E3    !(239,-
239)<RAnZI94>!
C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO   4.0E12      0.      17.5E3    !(240,-
240)<RAnZI94>!
C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO 6.8E11      0.      15.4E3    !(241,-
241)<RAnZI94>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!

!****** REACTIONS DE R15C2H5O ******!

!****** REACTIONS DE C2H5OH ******!

!Voir Plus bas meca 10a Luc Sy Tran

!****** REACTIONS DE O2 ******!
B1O+B1O+M=O2+M                  5.40E13     0.   -1.79E3    !(244,-
244)<BAULCH94>!
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
O2+R1H=R2OH+B1O                 9.8E13      0.     14.8E3    !(245,-
245)<BAULCH94>!
!O2+R1H+M=R3OOH+M                2.10E18    -0.8    0.00      !(246,-
246)<baseLeeds>!
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H+H2O=R3OOH+H2O            6.90E15    0.0    -2.10E3    !(246,-
246bis)<base Leeds>!

O2+R1H(+M)=R3OOH(+M)            4.52E13     0.       0.           !(246,-
246)<COBOS85>!
               LOW   /1.8E18     -0.8       0.00/                     !k0
BAULCH94!
               TROE  /0.5         1.0      1.0E8/
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H(+H2O)=R3OOH(+H2O)        1.63E14     0.       761.    !(246b,-
246b)<COBOS85>!
O2+R1H(+H2O)=R3OOH(+H2O)         4.52E13     0.         0.    !(246b,-
246b)<BAULCH94>!
               LOW   /6.9E15     0.0      -2080/
               TROE  /0.45       1.0      1.0E8/
O2+B3C=B2CO+B1O                 1.2E14      0.         0.     !(247,-
247)<RAnZI94>!
O2+B4CH=R5CHO+B1O                3.3E13      0.         0.    !(248,-
248)<DAGAUT91>!
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```
O2+B4CH=B2CO+R2OH              3.2E13      0.          0.   !(249,-
249)<PEETERS97>!
O2+B6CH2=>B2CO+R2OH+R1H        3.1E12      0.          0.   !
(250)<BAULCH94>!
O2+B5CH2=R5CHO+R2OH            4.3E10      0.      -0.5E3   !(251,-
251)<DAGAUT91>!
O2+B5CH2=CO2+H2                6.9E11      0.       0.5E3   !(252,-
252)<DAGAUT91>!
O2+B5CH2=>CO2+R1H+R1H          1.6E12      0.       1.0E3   !
(253)<DAGAUT91>!
O2+B5CH2=B2CO+H2O              1.9E10      0.      -1.0E3   !(254,-
254)<DAGAUT91>!
O2+B5CH2=>B2CO+R2OH+R1H        8.6E10      0.      -0.5E3   !
(255)<DAGAUT91>!
O2+B5CH2=HCHO+B1O              1.0E14      0.       4.5E3   !(256,-
256)<DAGAUT91>!
O2+R4CH3(+M)=R8CH3OO(+M)       7.8E8       1.2         0.   !(257,-
257)<BAULCH94>!
                    LOW   /5.6E25     -3.3         0./
                    TROE  /0.36        1.0       1.0E8/
O2+R4CH3=R7CH3O+B1O            1.3E14      0.      31.3E3   !(258,-
258)<BAULCH94>!
!O2+R4CH3=R7CH3O+B1O           1.6E13      0.      31.4E3   !(258,-
258)<HWAnG&RABInOVITCH99>!

O2+R4CH3=HCHO+R2OH             3.0E30     -4.69    36.6E3   !(259,-
259)<DAGAUT91>!
O2+CH4=R4CH3+R3OOH             4.0E13      0.      56.7E3   !(260,-
260)<BAULCH94>!
O2+R9C2H=B2CO+R5CHO            3.8E13     -0.16        0.   !(261,-
261)<TIESEMAnn97/TSAnG86>!
O2+R9C2H=R12CHCOZ+B1O          9.0E12     -0.16        0.   !(262,-
262)<TIESEMAnn97/TSAnG86>!
O2+C2H2=R9C2H+R3OOH            1.2E13      0.      74.5E3   !(263,-
263)<TSAnG86>!
!O2+C2H2=R12CHCOZ+R2OH         2.0E8       1.5     30.1E3   !(264,-
264)<DAGAUT91>!
O2+C2H2=R5CHO+R5CHO            7.0E7       1.8     30.6E3   !(264,-
264)<BEnSOn95>!

!O2+R10C2H3V=C2H2+R3OOH        1.2E11      0.          0.   !(265,-
265)<TSAnG86>!

!O2+R10C2H3V=C2H2+R3OOH        1.6E14     -0.83     2.5E3   !(265,-
265)<WAnG97>!
!at 760 Torr
!O2+R10C2H3V=HCHO+R5CHO        8.6E21     -2.97     3.3E3   !(266a,-
266a)<WAnG97>!
!O2+R10C2H3V=B1O+R13CH2CHO     1.2E13     -0.12     1.7E3   !(266b,-
266b)<WAnG97>!
!at 20-90 Torr
!O2+R10C2H3V=HCHO+R5CHO        1.6E21     -2.78     2.5E3   !(266a,-
266a)<WAnG97>!
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```
!O2+R10C2H3V=B1O+R13CH2CHO     2.5E12      0.057   0.9E3   !(266b,-
266b)<WAnG97>!

O2+R10C2H3V=C2H2+R3OOH         1.34E6      1.61   -0.4E3   !(265,-
265)<MEBEL nIST>!
O2+R10C2H3V=HCHO+R5CHO         4.5E16     -1.39    1.0E3   !(266a,-
266a)<MEBEL nIST>!
O2+R10C2H3V=B1O+R13CH2CHO      3.3E11     -0.29      10.   !(266b,-
266b)<MEBEL nIST>!

O2+C2H4Z=R10C2H3V+R3OOH        4.2E13      0.     57.4E3   !(267,-
267)<TSAnG86>!
O2+R11C2H5=R17C2H5OO          2.2E10      0.77   -0.6E3    !(268,-
268)<WAGnER90>!
O2+R11C2H5=C2H4Z+R3OOH         8.4E11      0.      3.9E3   !(269,-
269)<TSAnG86>!
O2+R11C2H5=R15C2H5O+B1O        1.2E13     -0.2    27.9E3   !(270,-
270)<BOZZELLI90nIST>!
O2+R11C2H5=CH3CHO+R2OH         6.0E10      0.      6.9E3   !(271,-
271)<TSAnG86>!
O2+C2H6=R11C2H5+R3OOH          6.0E13      0.     51.7E3   !(272,-
272)<BAULCH94>!
O2+R2OH=R3OOH+B1O              2.2E13      0.     52.5E3   !(273,-
273)<TSAnG86>!
O2+B2CO=CO2+B1O                2.5E12      0.     47.7E3   !(274,-
274)<TSAnG86>!
!O2+R5CHO=B2CO+R3OOH           5.1E13      0.      1.7E3   !(275,-
275)<TSAnG86>!
O2+R5CHO=B2CO+R3OOH            7.6E12      0.     0.41E3   !(275,-
275)<TIMOnEn88>!
O2+HCHO=R5CHO+R3OOH            2.0E13      0.     38.8E3   !(276,-
276)<TSAnG86)!
O2+R7CH3O=HCHO+R3OOH           2.2E10      0.      1.7E3   !(277,-
277)<BAULCH94>!
O2+R6CH2OH=HCHO+R3OOH          1.2E12      0.         0.   !(278,-
278)<TSAnG87>!
O2+CH3OH=R6CH2OH+R3OOH         2.0E13      0.     44.9E3   !(279,-
279)<TSAnG87>!
O2+R12CHCOZ=>B2CO+B2CO+R2OH    1.5E12      0.      2.5E3   !(280)
<DAGAUT91>!
!O2+CH2COZ=HCHO+CO2            1.0E8       0.         0.   !(281,-
281)<DAGAUT91>!bizarre
O2+R14CH3CO=R18CH3COOO        2.4E12      0.         0.    !(282,-
282)<COX90>!
O2+R13CH2CHO=>HCHO+R2OH+B2CO   5.9E9       0.     -1.4E3   !(283)
<COX90>!
O2+R13CH2CHO=CH2COZ+R3OOH      1.0E10      0.     -1.4E3   !(284,-
284)<COX90>!
O2+CH3CHO=R14CH3CO+R3OOH       5.0E13      0.     36.4E3   !(285,-
285)<COX90>!
! ajout demande par Laetitia le 25 Avril 95
O2+CH3CHO=R13CH2CHO+R3OOH      1.0E13      0.5    46.0E3   !(285',-
285)<Ranzi94>!
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O2+C2H4O#3=R3OOH+R13CH2CHO     5.0E13      0.     48.0E3   !(286,-
286)<RAnZI94>!
!O2+R15C2H5O=CH3CHO+R3OOH       6.0E10      0.      1.7E3  !(287,-
287)<BAULCH94>!

!****** REACTIONS DE R3OOH ******!
R3OOH+R1H=H2+O2                 4.3E13      0.      1.4E3  !(288,-
288)<BAULCH94>!
R3OOH+R1H=2R2OH                 1.7E14      0.      0.9E3  !(289,-
289)<BAULCH94>!
R3OOH+R1H=H2O+B1O               3.0E13      0.      1.7E3  !(290,-
290)<BAULCH94>!
R3OOH+B6CH2=HCHO+R2OH           3.0E13      0.         0.  !(291,-
291)<TSAnG86>!
R3OOH+B5CH2=HCHO+R2OH           1.8E13      0.         0.  !(292,-
292)<TSAnG86>!
R3OOH+R4CH3=R7CH3O+R2OH         1.8E13      0.         0.  !(293,-
293)<BAULCH94>!
!R3OOH+R4CH3=R7CH3O+R2OH        4.0E13      0.      5.0E3  !(293,-
293)<DAGAUT>
R3OOH+CH4=R4CH3+H2O2            9.0E12      0.     24.6E3  !(294,-
294)<BAULCH94>!
R3OOH+R9C2H=R12CHCOZ+R2OH       1.8E13      0.         0.  !(295,-
295)<TSAnG86>!
R3OOH+C2H2=CH2COZ+R2OH          6.0E9       0.      8.0E3  !(296,-
296)<TSAnG86>!
!incertitude au moins un facteur 10
R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO 3.0E13      0.         0.  !(297)
<TSAnG86>!
R3OOH+C2H4Z=CH3CHO+R2OH         6.0E9       0.      7.9E3  !(298,-
298)<TSAnG86>!
R3OOH+C2H4Z=C2H4O#3+R2OH        2.2E12      0.     17.2E3  !(299,-
299)<BAULCH94>!
R3OOH+R11C2H5=>R4CH3+HCHO+R2OH  2.4E13      0.         0.  !(300)
<TSAnG86>!
R3OOH+R11C2H5=C2H4Z+H2O2        3.0E11      0.         0.  !(301,-
301)<TSAnG86>!
R3OOH+C2H6=R11C2H5+H2O2         1.3E13      0.     20.4E3  !(302,-
302)<BAULCH94>!
R3OOH+R2OH=H2O+O2               2.9E13      0.     -0.5E3  !(303,-
303)<BAULCH94>!
R3OOH+B2CO=CO2+R2OH             1.57E05     2.18   17.9E3  !MF Wang, J.
Phys. Chem. A 111(2007)4031 - 4042
R3OOH+R5CHO=>R2OH+R1H+CO2       3.0E13      0.         0.  !(305)
<TSAnG86>!
R3OOH+HCHO=R5CHO+H2O2           3.0E12      0.     13.0E3  !(306,-
306)<BAULCH94>!
R3OOH+R7CH3O=HCHO+H2O2          3.0E11      0.         0.  !(307,-
307)<TSAnG86>!
R3OOH+R6CH2OH=HCHO+H2O2         1.2E13      0.         0.  !(308,-
308)<TSAnG87>!
R3OOH+CH3OH=R6CH2OH+H2O2        9.6E10      0.     12.6E3  !(309,-
309)<TSAnG87>!
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R3OOH+R14CH3CO=>R4CH3+CO2+R2OH  3.0E13      0.          0.  !
(310)<TSAnG86>!
R3OOH+CH3CHO=R14CH3CO+H2O2      1.0E12      0.     10.0E3  !(311,-
311)<CAVAnAGH90>!
R3OOH+C2H4O#3=H2O2+R13CH2CHO    1.6E12      0.     15.0E3  !(312,-
312)<RAnZI94>
R3OOH+R3OOH=H2O2+O2             1.3E11      0.    -1.63E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE
R3OOH+R3OOH=H2O2+O2             4.2E14      0.    11.98E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE

!****** REACTIONS DE H2O2 ******!
!R2OH+R2OH(+ M)=>H2O2 (+ M)     7.23E13    -0.37    0.00
!       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /5.53E19  -0.76     0.00 /
!        TROE /0.5 1 1.E8/
!H2O2(+M)=>R2OH+R2OH(+M)         3.00E14     0.00    48.5E3
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /3.0E17   0.0     45.5E3/
!       TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601
H2O2(+M)=R2OH+R2OH(+M)        1.99E12     0.9    4.8749E4 !<BAULCH94>!
          AR/0.68/ O2/0.79/ N2/1.00/ CO2/1.06/ H2O/5.1/ H2O2/5.2/
        LOW  /3.65e24   -2.3   4.8749E4/
        TROE /0.43 1 1.E8/

H2O2+R1H=H2+R3OOH               1.7E12      0.      3.7E3   !(315,-
315)<BAULCH94>!
H2O2+R1H=H2O+R2OH               1.0E13      0.      3.6E3   !(316,-
316)<BAULCH94>!
H2O2+B6CH2=R7CH3O+R2OH          3.0E13      0.         0.   !(317,-
317)<TSAnG86>!
H2O2+R10C2H3V=C2H4Z+R3OOH       1.2E10      0.     -0.6E3   !(318,-
318)<TSAnG86>!
H2O2+B1O=R2OH+R3OOH             6.6E11      0.      4.0E3   !(319,-
319)<BAULCH94>!
H2O2+R2OH=H2O+R3OOH             7.8E12      0.      1.3E3   !(320,-
320)<BAULCH94>!

!****** REACTIONS DE CO2 ******!
CO2+B5CH2=HCHO+B2CO             2.3E10      0.         0.   !(321,-
321)<TSAnG86>!

!****** REACTIONS DE R8CH3OO ******!
R8CH3OO=HCHO+R2OH                 1.5E13      0.     47.0E3 !(322,-
322)<RAnZI94>!
R8CH3OO+R1H=R7CH3O+R2OH           9.6E13      0.         0. !(323,-
323)<TSAnG86>!
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R8CH3OO+H2=CH3OOH+R1H              3.0E13      0.     26.0E3 !(324,-
324)<TSAnG86>!
R8CH3OO+B6CH2=HCHO+R7CH3O          1.8E13      0.         0. !(325,-
325)<TSAnG86>!
R8CH3OO+B5CH2=HCHO+R7CH3O          1.8E13      0.         0. !(326,-
326)<TSAnG86>!
R8CH3OO+R4CH3=R7CH3O+R7CH3O        5.0E12      0.     -1.4E3 !(327,-
327)<CAVAnAGH90>!
R8CH3OO+CH4=CH3OOH+R4CH3           1.8E11      0.     18.5E3 !(328,-
328)<TSAnG86>!
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ      2.4E13      0.         0. !(329,-
329)<TSAnG86>!
!R8CH3OO+C2H2=CH3OOH+R9C2H          5.6E11      0.     24.5E3 !(330,-
330)<RAnZI94>! MF car i<<0
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 2.4E13      0.         0. !(331,-
331)<TSAnG86*>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3       1.1E15      0.     20.0E3 !(332,-
332)<nIKISHA81/MOSHKInA80nIST>!
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V      3.9E12      0.     24.5E3 !(333,-
333)<RAnZI94>!
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O    2.4E13      0.         0. !(334,-
334)<TSAnG86>!
R8CH3OO+C2H6=CH3OOH+R11C2H5        2.9E11      0.     14.9E3 !(335,-
335)<TSAnG86>!
R8CH3OO+B1O=R7CH3O+O2              3.6E13      0.         0. !(336,-
336)<TSAnG86>!
R8CH3OO+R2OH=CH3OH+O2              6.0E13      0.         0. !(337,-
337)<TSAnG86>!
R8CH3OO+R2OH=R7CH3O+R3OOH          3.0E12      0.         0. !(338,-
338)<RAnZI94>!
R8CH3OO+B2CO=R7CH3O+CO2            1.0E14      0.     24.0E3 !(339,-
339)<RAnZI94>!
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2      3.0E13      0.         0. !(340)
<TSAnG86>!
R8CH3OO+HCHO=CH3OOH+R5CHO          1.0E12      0.     12.1E3 !(341,-
341)<CAVAnAGH90>!
R8CH3OO+R7CH3O=HCHO+CH3OOH         3.0E11      0.         0. !(342,-
342)<TSAnG86>!
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO 1.2E13      0.         0. !
(343)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R6CH2OH       1.8E12      0.     13.7E3 !(344,-
344)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R7CH3O        2.8E11      0.     18.8E3 !(345,-
345)<RAnZI94>!
R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ     1.7E12      0.     27.0E3 !(346,-
346)<RAnZI94>!
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O  2.4E13      0.         0. !(347,-
347)<TSAnG86>!
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO     1.0E12      0.     12.1E3 !(348,-
348)<CAVAnAGH90>!
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO    1.7E12      0.     19.2E3 !(349,-
349)<RAnZI94>!
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R8CH3OO+C2H4O#3=CH3OOH+R13CH2CHO  2.2E12      0.     16.0E3 !(350,-
350)<RAnZI94>!
R8CH3OO+R3OOH=CH3OOH+O2           2.5E11      0.     -1.6E3 !(351,-
351)<BAULCH94>!
R8CH3OO+R3OOH=>O2+HCHO+H2O        5.0E10      0.         0. !
(352)<RAnZI94>!
R8CH3OO+H2O2=CH3OOH+R3OOH         2.4E12      0.      9.9E3 !(353,-
353)<TSAnG86>!
R8CH3OO+R8CH3OO=CH3OH+HCHO+O2     2.5E10      0.     -0.8E3 !(354,-
354)<BAULCH94>!
R8CH3OO+R8CH3OO=R7CH3O+R7CH3O+O2  2.5E10      0.     -0.8E3 !(355,-
355)<BAULCH94>!

!****** REACTIOnS DE CH3OOH ******!
CH3OOH=R7CH3O+R2OH               6.0E14      0.     42.3E3 !(356,-
356)<BAULCH94>!
CH3OOH+B1O=R8CH3OO+R2OH          2.0E13      0.      4.8E3 !(357,-
357)<BAULCH94average>!
CH3OOH+R2OH=H2O+R8CH3OO          1.8E12      0.    -0.37E3 !(358,-
358)<BAULCH94average>!
CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO   1.5E11      0.      6.5E3 !
(359)<RAnZI94>!

!****** REACTIOnS DE R17C2H5OO ******!
R17C2H5OO=R16C2H4OOH               4.2E12      0.     36.9E3 !(360,-
360)<HUGHES93>!
R17C2H5OO+H2=C2H5OOH+R1H           7.9E12      0.     21.0E3 !(361,-
361)<RAnZI94>!
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O    2.0E12      0.     -1.2E3 !(362,-
362)<RAnZI94>!
R17C2H5OO+CH4=C2H5OOH+R4CH3        3.9E12      0.     24.0E3 !(363,-
363)<RAnZI94>!
R17C2H5OO+C2H2=C2H5OOH+R9C2H       5.6E11      0.     24.4E3 !(364,-
364)<RAnZI94>!
R17C2H5OO+C2H4Z=C2H5OOH+R10C2H3V   3.9E12      0.     24.4E3 !(365,-
365)<RAnZI94>!
R17C2H5OO+C2H4Z=R15C2H5O+C2H4O#3   2.3E16      0.     21.9E3 !(366,-
366)<MOSHKInA80nIST>!
R17C2H5OO+C2H6=C2H5OOH+R11C2H5     5.1E12      0.     19.5E3 !(367,-
367)<RAnZI94>!
R17C2H5OO+H2O=C2H5OOH+R2OH         5.6E12      0.     30.6E3 !(368,-
368)<RAnZI94>!
R17C2H5OO+B2CO=CO2+R15C2H5O        1.0E14      0.     24.0E3 !(369,-
369)<RAnZI94>!
R17C2H5OO+HCHO=C2H5OOH+R5CHO       4.5E12      0.     14.4E3 !(370,-
370)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R7CH3O     2.8E11      0.     18.4E3 !(371,-
371)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R6CH2OH    2.8E12      0.     19.5E3 !(372,-
372)<RAnZI94>!
R17C2H5OO+CH2COZ=C2H5OOH+R12CHCOZ  1.7E12      0.     24.4E3 !(373,-
373)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R14CH3CO  3.9E12      0.     14.4E3 !(374,-
374)<RAnZI94>!
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R17C2H5OO+CH3CHO=C2H5OOH+R13CH2CHO 1.7E12      0.     19.5E3 !(375,-
375)<RAnZI94>!
R17C2H5OO+C2H4O#3=C2H5OOH+R13CH2CHO 2.2E12      0.     16.3E3 !(376,-
376)<RAnZI94>!
R17C2H5OO+R3OOH=O2+C2H5OOH         3.9E11      0.     -1.3E3 !(377,-
377)<BAULCH89>!
!Rate constant measured between 240 and 380K!
R17C2H5OO+H2O2=C2H5OOH+R3OOH       4.5E11      0.     10.8E3 !(378,-
378)<RAnZI94>!
R17C2H5OO+R8CH3OO=>R15C2H5O+R7CH3O+O2  2.0E11      0.         0. !
(379)<RAnZI94>!
R17C2H5OO+CH3OOH=C2H5OOH+R8CH3OO   1.1E12      0.     16.3E3 !(380,-
380)<RAnZI94>!
R17C2H5OO+R17C2H5OO=2R15C2H5O+O2   4.1E10      0.      0.2E3 !(381,-
381)<LIGHTFOOT92>!
R17C2H5OO+R17C2H5OO=C2H5OH+CH3CHO+O2  1.8E10      0.       0.2E3 !(382,-
382)<LIGHTFOOT92>!

!****** REACTIONS DE R16C2H4OOH ******!
R16C2H4OOH=C2H4O#3+R2OH            1.5E11      0.     20.0E3 !(383,-
383)<RAnZI94>!
R16C2H4OOH=R6CH2OH+HCHO            2.5E13      0.     27.5E3 !(384,-
384)<RAnZI94>!
R16C2H4OOH=C2H4Z+R3OOH             2.0E13      0.     23.5E3 !(385,-
385)<RAnZI94>!

!****** REACTIONS DE C2H5OOH ******!
C2H5OOH=R15C2H5O+R2OH               4.0E15      0.     42.9E3 !(386,-
386)<BAULCH94>!
C2H5OOH+R1H=>CH3CHO+R2OH+H2         3.2E13      0.      7.7E3 !
(387)<RAnZI94>!
C2H5OOH+R4CH3=>CH3CHO+R2OH+CH4      5.7E11      0.      8.7E3 !
(388)<RAnZI94>!
C2H5OOH+R9C2H=>CH3CHO+R2OH+C2H2     6.0E11      0.      9.2E3 !
(389)<RAnZI94>!
C2H5OOH+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12      0.      8.7E3 !
(390)<RAnZI94>!
C2H5OOH+R11C2H5=>CH3CHO+R2OH+C2H6   3.4E11      0.     11.4E3 !
(391)<RAnZI94>!
C2H5OOH+R2OH=>CH3CHO+R2OH+H2O       5.9E12      0.      0.9E3 !
(392)<RAnZI94>!
C2H5OOH+R5CHO=>CH3CHO+R2OH+HCHO     1.8E12      0.     16.7E3 !
(393)<RAnZI94>!
C2H5OOH+R7CH3O=>CH3CHO+R2OH+CH3OH   6.3E11      0.      5.5E3 !
(394)<RAnZI94>!
C2H5OOH+R6CH2OH=>CH3CHO+R2OH+CH3OH  4.2E11      0.     13.6E3 !
(395)<RAnZI94>!
C2H5OOH+R14CH3CO=>2CH3CHO+R2OH      2.0E12      0.     18.5E3 !
(396)<RAnZI94>!
C2H5OOH+R13CH2CHO=>2CH3CHO+R2OH     3.4E11      0.     15.7E3 !
(397)<RAnZI94>!
C2H5OOH+R3OOH=>CH3CHO+R2OH+H2O2     8.0E11      0.     16.2E3 !
(398)<RAnZI94>!
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C2H5OOH+R8CH3OO=>CH3CHO+R2OH+CH3OOH 1.1E12      0.     16.7E3 !
(399)<RAnZI94>!
C2H5OOH+R17C2H5OO=>CH3CHO+R2OH+C2H5OOH  1.1E12      0.     16.7E3 !
(400)<RAnZI94>!

!****** REACTIONS DE R18CH3COOO ****** !
R18CH3COOO+C2H4O#3=CH3COOOH+R13CH2CHO     1.0E12      0.      9.3E3 !
(401,-402)<RAnZI94>!
R18CH3COOO+R3OOH=CH3COOOH+O2              5.5E10      0.     -2.6E3 !
(402,-402)<COX90>!
R18CH3COOO+C2H5OOH=CH3COOOH+R17C2H5OO     5.0E11      0.      9.2E3 !
(403,-403)<RAnZI94>!
R18CH3COOO+C2H5OOH=>CH3CHO+R2OH+CH3COOOH  5.0E11      0.      9.2E3 !
(404)<RAnZI94>!
R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2     1.7E12      0.     -1.0E3 !
(405)<CAVAnAGH90>!

!****** REACTIONS DE CH3COOOH ******!
CH3COOOH=>R4CH3+CO2+R2OH                  1.0E16      0.     40.0E3 !
(406)<CAVAnAGH90>!

!*********************************************************

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!*                                          Primary mechanism of the
oxidation of Ethanol                                        *!
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!*************************************!
!*           REACTIOnS OF ETHANOL      *!
!*************************************!

!Unimolecular initiation

C2H5OH(+M)=R11C2H5+R2OH(+M)       2.95E+22    -2.16        96.6E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /3.80E+88   -19.70       114.5E+3/
                          TROE   /2.094   16539    1.114   161.36/

C2H5OH(+M)=C2H4Z+H2O(+M)          4.90E+9     1.36    65.8E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /2.404+8    -17.9    84.8E+3/
                          TROE   /2.126     13568   0.969  160.4/
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C2H5OH(+M)=R4CH3+R6CH2OH(+M)     6.61E+23  -2.16    88.04E+3
!Tsang, J Chem Kinet 36,436-63,2004!
                          LOW     /1.99E+85  -18.9    104.8E+3/
                          TROE    /2.058     16911    1.071   135.3/

C2H5OH(+M)=R23C2H4OH+R1H(+M)     2.01E+17    -0.149     101.8E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                          LOW     /4.902E+94   -21.65     123.1E+3/
!Reaction (c5),T=500-1800K
                         !LOW     /2.716E+83   -21.47     38.44E+3/
!Reaction (c5),T=1800-3000K

C2H5OH(+M)=R24C2H4OH+R1H(+M)     7.54E+16    -0.275   94.05E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                          LOW     /7.708E+96   -22.47   116.9E+3/
!T=500-1800K
                         !LOW     /5.58E+82    -21.20   37824.5/
!T=1800-3000K
                          DUPLICATE

C2H5OH(+M)=R15C2H5O+R1H(+M)      2.70E+15    0.305    101.3E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!
                         LOW      /2.794E+88  -19.76    121.0E+3/
!T=500-1800K;
                        !LOW      /4.246E+91  -23.49    49435.8/
!T=1800-3000K,
                         DUPLICATE

!Bimolecular initiation

C2H5OH+O2=R23C2H4OH+R3OOH           2.100E+13      0.0     52400.0
C2H5OH+O2=R24C2H4OH+R3OOH           1.400E+13      0.0     46300.0
C2H5OH+O2=R15C2H5O+R3OOH            7.000E+12      0.0     55730.0

!Metatheses with abstraction of H-atom

!C2H5OH+R2OH=R23C2H4OH+H2O              6.203E+03      2.68      -576.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R23C2H4OH+H2O               3.60E+06       2.0        950.0
!Nancy, correlation Bozzelli 1999!

!C2H5OH+R2OH=R24C2H4OH+H2O              1.307E+05      2.43     -1456.6
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R24C2H4OH+H2O               2.40E+06       2.00     -2100.0
!Nancy, correlation Bozzelli 1999!

C2H5OH+R2OH=R15C2H5O+H2O                2.812E+02      2.97     -580.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H5OH+B1O=R23C2H4OH+R2OH               9.69E+02       3.23     4658.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007
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C2H5OH+B1O=R24C2H4OH+R2OH                1.45E+05       2.47     876.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H5OH+B1O=R15C2H5O+R2OH                 1.46E-03       4.73     1727.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H5OH+R1H=R23C2H4OH+H2                  1.88E+03       3.20     7150.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R24C2H4OH+H2                  1.79E+05       2.53     3420.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R15C2H5O+H2                   5.33E-23       10.58    -4459.0
!T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).
!C2H5OH+R1H=R15C2H5O+H2                  5.36E+4        2.53     8753.6
!T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

!C2H5OH+R4CH3=R23C2H4OH+CH4              6.99E-83      30.14   -15663.0
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R23C2H4OH+CH4               3.30E+02       3.30    12291.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).

!C2H5OH+R4CH3=R24C2H4OH+CH4              1.02E-47      18.51    -9409.4
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R24C2H4OH+CH4               1.99E+01      3.37     7635.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

!C2H5OH+R4CH3=R15C2H5O+CH4               1.01E-51      19.68    -10323.5
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R15C2H5O+CH4                2.035E+0      3.57     7722.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

C2H5OH+R3OOH=R23C2H4OH+H2O2              4.2E+04        2.69     19080
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R24C2H4OH+H2O2              2.80E+04       2.69     15420
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R15C2H5O+H2O2           5.400E+04      2.0     15025.0    !
Grana et al.2010

C2H5OH+R11C2H5=R23C2H4OH+C2H6        1.500E+12      0.0     11700.0    !
Konnov 2005!

C2H5OH+R11C2H5=R24C2H4OH+C2H6        4.000E+13      0.0     10000.0    !
Konnov 2005!

C2H5OH+R11C2H5=R15C2H5O+C2H6         2.300E+04      2.0     10525.0    !
Grana et al.2010!

C2H5OH+R6CH2OH=R24C2H4OH+CH3OH       4.000E+11      0.0      9700.0    !
Konnov 2005!
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C2H5OH+R7CH3O=R24C2H4OH+CH3OH         2.000E+11      0.0      7000.0    !
Konnov 2005!

C2H5OH+R15C2H5O=C2H5OH+R24C2H4OH      2.000E+11      0.0      7000.0    !
Konnov 2005!


!****************************************!
!*           REACTIOnS OF R23C2H4OH     *!
!****************************************!

R23C2H4OH=C2H4Z+R2OH                        3.52E-34      11.84   -18737.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                           1.35E+43      -10.29    28035.5
!at 1 atm, T=300-1000K
!                                           7.93E+2        1.51     15180.3
!at 1 Torr, T=300-3000K
!                                           1.51E+33      -6.54     26960.4
!at 100 atm, T=300-1000K
!                                           4.90E-24       9.44    -12183.6
!at 100 atm, T=1000-3000K

R23C2H4OH=R1H+C2H3OH                        3.33E+28      -5.26    35586.9
!at 1 atm,T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                           2.67E+15      -1.92    29386.8
!at 1 Torr,T=300-3000K.
!                                           2.67E+27      -4.44    37208.5
!at 100 atm,T=300-3000K

R23C2H4OH=R24C2H4OH                      1.000E+11      0.0     39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81


R23C2H4OH+O2=C2H3OH+R3OOH        1.600E+12      0.0     5000.0

!****************************************!
!*           REACTIOnS OF R24C2H4OH     *!
!****************************************!

R24C2H4OH=CH3CHO+R1H                        8.34E+27       -5.19    35576.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                          8.96E+13       -1.61    28844.3
!at 1 Torr,T=300-3000K
!!                                          5.47E+27       -4.67    37685.4
!at 100 atm,T=300-3000K

R24C2H4OH=R1H+C2H3OH                        2.00E+28      -5.08    39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                          4.44E+21      -3.23    36570.6
!at 1 Torr,T=300-3000K
!!                                          1.22E+30      -5.17    41916.2
!at 100 atm,T=300-3000K
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R24C2H4OH=R4CH3+HCHO                    1.14E+22       -3.59   34662.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                      5.92E+11       -1.04   28739.0
!at 1 Torr,T=300-3000K
!!                                      4.36E+23       -3.55   38679.0
!at 100 atm,T=300-3000K

R24C2H4OH+O2=CH3CHO+R3OOH               5.26E+17       -1.637   838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=CH3CHO+R3OOH             5.28E+17       -1.637   839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.

R24C2H4OH+O2=C2H3OH+R3OOH               5.33E+2        2.490    -402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=C2H3OH+R3OOH             7.62E+2        2.446    -296
!at 1 atm, T=300-2000K,Ref: DaSilva et al 2009, JphyschemA, 113,31.

R24C2H4OH+R1H=CH3CHO+H2                 1.361E+09     1.29        2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=R6CH2OH+R4CH3             8.67E+16      -0.891      2903.3
!Rйaction (b2), Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=C2H3OH+H2                 4.896E+08      1.70       588.2
!Rйaction (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-
22.

R24C2H4OH+R1H(+M)=C2H5OH(+M)            3.607E+13       0.06      437.2
!Rйaction (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,
                                  LOW /2.767E+56     -15.72
10.7E+03/
                                 Duplicate

R24C2H4OH+R2OH=CH3CHO+H2O            1.500E+13      0.0         0.0
!Konnov 2005

R24C2H4OH+B1O=CH3CHO+R2OH                9.040E+13      0.0         0.0
!Konnov 2005

!*************************************!
!*           REACTIOnS OF R15C2H5O     *!
!*************************************!

R15C2H5O=R4CH3+HCHO                      4.4E-29      10.69   -16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                      1.03E+23    -3.82     19303.7
!at 1 atm, T=300-1000K,
!!                                      2.71E+24    -4.50     21018.7
!at 1 Torr, T=300-1000K,
!!                                      1.87E-28    10.39    -12910.9
!at 1 Torr, T=1000-3000K,
!!                                      5.31E+21    -2.97     19560.1
!at 100 atm, T=300-1000K,
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!!                                        9.56E-17    7.66     -7408.3
!at 100 atm, T=1000-3000K,

R15C2H5O=R1H+CH3CHO                       4.25E-32     11.49    -16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                        1.33E+38     -8.61    25513.8
!at 1 atm,T=300-1000K
!!                                        7.25E+31     -7.58    21370.4
!at 1 Torr,T=300-1000K
!!                                        2.14E-34     11.63    -15651.2
!at 1 Torr,T=1000-3000K
!!                                        2.61E+19     -2.15    21996.4
!at 100 atm,T=300-1000K
!!                                        1.64E-27     10.5     -15315.4
!at 100 atm,T=1000-3000K

R15C2H5O+O2=CH3CHO+R3OOH                 6.0E+10       0.0        1.7E+3
!(287,-287)<BAULCH94>!

R15C2H5O+R2OH=CH3CHO+H2O                 1.0E+13       0.0        0.0
!Marinov 1998

R15C2H5O+R1H=CH3CHO+H2                   7.47E+09      1.15       673.7
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22

R15C2H5O+R1H(+M)=C2H5OH(+M)              3.08E+11      0.894      12.9
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22
                                    LOW / 3.772E+51    -15.55
11.1E+3/
                                    DUPLICATE

R15C2H5O+B1O=CH3CHO+R2OH                 1.210E+14     0.0        0.0
!Konnov 2005


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!*                                        Secondary mechanism of the
oxidation of Ethanol                                *!
!
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*************************************************!
!
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*************************************************!

!*************************************!
!*           REACTIONS OF C2H3OH       *!
!*************************************!
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!C2H3OH+B1O=R13CH2CHO+R2OH              4.4E+10       0.7       3250.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+B1O=R13CH2CHO+R2OH               1.4E+13       0.0       2.3E3
!Acйtaldйhyde! (219,-219)<CAVAnAGH90>

!C2H3OH+R1H=R13CH2CHO+H2              2.700E+04     2.5
-1900.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R1H=R13CH2CHO+H2              1477.2        3.077
7230       !T=300-3000!RAO 2011! J Phys Chem 2011,115
!                                  REV   /1.41         3.721     24600/
C2H3OH+R1H=R13CH2CHO+H2                 1.31E+5       2.58      1220.0
!Acйtaldйhyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem
A,114,755-764.

!C2H3OH+R2OH=R13CH2CHO+H2O            1.500E+06     2.0
-1520.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R2OH=R13CH2CHO+H2O               2.300E+10     0.73     -1100.0
!Acйtaldйhyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2          3.200E+03     2.6
12400.0    !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R3OOH=R13CH2CHO+H2O2          1.626E+12     0.0
16295.1    !Syn_CH2H3OH! ajoutй le 20/10/2011 !Altarawneh et al 2011!
T=700-1300K!
C2H3OH+R3OOH=R13CH2CHO+H2O2             1.0E12        0.0       10.0E3
!Acйtaldйhyde!(311,-311)<CAVAnAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4           5.000E+10     0.0
7300.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R4CH3=R13CH2CHO+CH4              2.0E-6        5.6       2.5E+3
!Acйtaldйhyde! (216,-216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6             0.740         3.5       4140.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+R11C2H5=R13CH2CHO+C2H6           1.3E12        0.0       8.5E3
!Acйtaldйhyde! (218,-218)<HOHLEIn70>

C2H3OH=CH3CHO                           4.5E+06       1.8       5.1E+4
!Prof. Fournet
!!C2H3OH=CH3CHO                         8.590E+11     0.318     55900.00
! DaSilva 2006!
  !!                              REV/   1.050E+09     1.202
66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH              1.49E+05      1.67      6810.0
!P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29
C2H3OH+R1H=CH3CHO+R1H                   1.00E+13      0.00      1506.0
!T=300-2000K!form observation in Huynh et al 2009, j phys chem A
113,3177-3185:
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!"The rate of this reaction is close to that of the H addition to C2H4:
C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+CO2+H2                1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5
!C2H3OH+R2OH=HCHO+R6CH2OH                1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5

!C2H4+OH<=>C2H3OH+H                      1.070E+04    2.600     4133.00
!Senosiain et al 2006
C2H4Z+R2OH=C2H3OH+R1H                    4.000E+12    0.000     4880.00
!Hippler et al 2000

!*************************************!
!*           REACTIOnS OF CH3CHO       *!
!*************************************!

CH3CHO+R2OH=R14CH3CO+H2O                 2.300E+10   0.73
-1100.0     ! Konnov 2005!
CH3CHO+R1H=H2+R14CH3CO                   1.31E+5     2.58
1220.0      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
CH3CHO+R4CH3=R14CH3CO+CH4                2.0E-6      5.6
2.5E+3      !(216,-216)<BAULCH94>! T=300-1250K
CH3CHO+B1O=R14CH3CO+R2OH                 1.4E+13     0.
2.3E3       !(219,-219)<CAVAnAGH90>!
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO           8.1E10      0.
3.7E3       !(217,-217)<SCHERZER87>T=480-520K!NIST
CH3CHO+R11C2H5=C2H6+R14CH3CO             1.3E12      0.
8.5E3       !(218,-218)<HOHLEIn70>!
CH3CHO+R7CH3O=R14CH3CO+CH3OH             5.000E+12   0.0
0.0         !Konnov 2005!
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO         3.000E+12   0.0
11200.0     !Konnov 2005!

!CH3CHO+R2OH=R13CH2CHO+H2O               1.600E+13   0.0
2000.0      !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J
Chem Kin 2008,40,73-102
CH3CHO+R2OH=R13CH2CHO+H2O                3.370e+11   0.0
-619.98     !Mech Sandiego=ref:Juan Li's PhD thesis!
!CH3CHO+R1H=R13CH2CHO+H2                 4.40E+14    0.0
10.0E+3     !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R1H=R13CH2CHO+H2                  2.72E+03    3.1
5206.5      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
!CH3CHO+R4CH3=R13CH2CHO+CH4              6.00E+12    0.0
11000.0     !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R4CH3=R13CH2CHO+CH4               2.45E+1     3.15
5727.0      !Marinov 1998
CH3CHO+B1O=R13CH2CHO+R2OH                3.720E+13   -0.2
3556.0      !Marinov 1998
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!****** REACTIONS DE C2H5 ******!
R11C2H5+R10C2H3V=>C4H8Y                    1.5E13      0.          0. !
(61,-61)<TSAnG86>!
!R11C2H5+R11C2H5=>C4H10                     1.1E13      0.          0. !
(65,-65)<BAULCH94>!


!****** REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE ******!

C2H3CHO+R2OH=CH2CHCO+H2O                   1.0E13      0.0    0.0    !
<MARInOV>!
C2H3CHO+B1O=CH2CHCO+R2OH                   7.2E12      0.0    2.0E3  !
<MARInOV>!
C2H3CHO+B1O=CH2COZ+R5CHO+R1H               5.0E7       1.76   0.08E3 !
<MARInOV>!
C2H3CHO+R1H=CH2CHCO+H2                     4.0E13      0.0    4.2E3  !
<MARInOV>!
C2H3CHO+R1H=C2H4Z+R5CHO                    2.0E13      0.0    3.5E3  !
<MARInOV>!
C2H3CHO+O2=CH2CHCO+R3OOH                   3.0E13      0.0   38.5E3  !
<MARInOV99>+ MF correlation Baptiste
CH2CHCO=R10C2H3V+B2CO                      1.0E14      0.0   34.0E3  !
<MARInOV>!
CH2CHCO+B1O=R10C2H3V+CO2                   1.0E14      0.0    0.0    !
<MARInOV>!
C3H5Y+R3OOH=>C2H3CHO+R1H+R2OH               7.0E18     -2.0    0.0    !
<TSAnG91>!
C3H5Y+O2=C2H3CHO+R2OH                      1.8E13     -0.41   22.9E3 !
<BOZELLI93>!
C3H5Y+B1O=C2H3CHO+R1H                      1.8E14      0.0     0.0   !
<SLAGLE92>!

!*****************************************************!
!       REACTIONS DES ESPECES NON OXYGEnNS EN C3      !
!*****************************************************!

!****** REACTIONS DE C3H2  ***** (CHCCH(..))*****!

B4CH+C2H2=C3H2+R1H                        2.1E14       0.0        -0.5E3 !
<MILLER92/BAULCH94>!
C3H2+B1O=R9C2H+R1H+B2CO                   3.0E13       0.0         0.0   !
<PEETERS97>!
C3H2+R2OH=C2H2+R5CHO                      5.0E13       0.0         0.0   !
<MILLER92>!
C3H2+O2=R12CHCOZ+B2CO+R1H                 5.0E13       0.0         0.0   !
<MILLER92>!


!****** REACTIONS DE C3H3 ***** (CHCCH2(.)) Propargyl*****stablilise par
resonnance !
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B6CH2+C2H2=C3H3+R1H                    1.8E14       0.0          0.0   !
<MILLER87/BAULCH94>!
C3H3+R1H=C3H2+H2                       2.0E13       0.0          0.0   !
<MILLER92/BRAUn89>!
C3H3+B1O=R9C2H+HCHO                    1.4E14       0.0          0.0   !
<MILLER92/SLAGUE91>!
C3H3+R2OH=C3H2+H2O                     2.0E13       0.0          0.0   !
<MILLER92>!
C3H3+R2OH=R10C2H3V+R5CHO               4.0E13       0.0          0.0   !
<WAnG97>!
C2H2+R12CHCOZ=C3H3+B2CO                1.0E11       0.0          3.0E3 !
<MILLER92>!
C3H3+O2=CH2COZ+R5CHO                   3.0E10       0.0          2.9E3 !
<MILLER92/SLAGUE88>!
C3H2+R1H=C3H3                          1.0E14       0.0          0.0   !
<est>!
C3H3+R3OOH=>R2OH+R9C2H+HCHO             1.0E15      -0.8          0.0   !
<Heyberger>!
C3H3+C3H3=C6H6#                       1.0E12       0.0          0.0   !
<STEIn90>shocktube!
C3H3+C3H3=C6H5#+R1H                    1.0E12       0.0          0.0   !
<STEIn90>flame!



!****** REACTIONS DE pC3H4 ***** (CH3CCH) Propyne *****!

!pC3H4=>aC3H4                           2.1E12       0.0         60.0E3
     !<HIDAKA89>!
pC3H4+M=C3H3+R1H+M                     4.7E18       0.0         80.0E3
     !<HIDAKA89>!
C2H2+B5CH2=pC3H4                       3.5E12       0.0          0.0
     !<TSAnG86>!

pC3H4=R9C2H+R4CH3                      4.2E15       0.0        125.0E3  !
<KInGAS1500>!
pC3H4+O2=C3H3+R3OOH                    2.1E12       0.0         40.8E3  !
<est Ingham>!
pC3H4+R1H=C2H2+R4CH3                   1.3E5        2.5         1.00E3  !
<hidaka89> !
pC3H4+R1H(+M)=tC3H5(+M)                8.5E12       0.0         1.7E3   !
<WAGnER72>!
                    LOW   /5.6E25     -7.27     6.58E3/
          !<Marinov97!
pC3H4+R1H(+M)=sC3H5(+M)                5.8E12       0.0         3.1E3   !
     <WAGnER72>!
                    LOW   /3.8E25     -7.27     7.98E3/
          !<estimated>!
pC3H4+R4CH3=C3H3+CH4                   2.2E0        3.5         5.7E3   !
<asTSAnG91>!
pC3H4+R1H=C3H3+H2                      1.7E5        2.5         2.5E3   !
<asTSAnG91>
```

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pC3H4+R9C2H=C3H3+C2H2                    3.6E12      0.0           0.0
     !<asTSAnG91>!
pC3H4+R10C2H3V=C3H3+C2H4Z                2.2E0       3.5          4.7E3  !
<asTSAnG91>!
pC3H4+R11C2H5=C3H3+C2H6                  2.2E0       3.5          6.6E3  !
<asTSAnG91>!
pC3H4+B1O=R12CHCOZ+R4CH3                 1.5E13      0.0          2.1E3  !
<WARnATZ84>!
pC3H4+B1O=R2OH+C3H3                      3.4E4       2.16         4.8E3  !
<<ADUSEI, G.Y, 1996>!
pC3H4+R2OH=CH2COZ+R4CH3                  4.3E11      0.0         -0.8E3  !
<BOODAGHIAnS87>!
pC3H4+R2OH=R1H+C2H3CHO                   4.3E11      0.0         -0.8E3  !
<asBOODAGHIAnS87>!
pC3H4+R2OH=C3H3+H2O                      3.1E6       2.0         -0.3E3  !
<asTSAnG91>!
pC3H4+R3OOH=C2H4Z+B2CO+R2OH              6.0E9       0.0          8.0E3  !
as296<TSAnG86>!
pC3H4+R3OOH=C3H3+H2O2                    9.6E3       2.6         13.9E3  !
<asTSAnG91>!
pC3H4+R7CH3O=CH3OH+C3H3                  2.0E12      0.0          4.0E3  !
<Heyberger>!


!******** REACTIONS DE aC3H4 ***** (CH2CCH2) Allene  *******!

aC3H4=pC3H4                              2.5E12      0.0         59.0E3  !
<HIDAKA89>!
aC3H4+M=C3H3+R1H+M                       2.0E18      0.0         80.0E3  !
<HIDAKA89>!
aC3H4+O2=C3H3+R3OOH                      2.8E13      0.0         39.0E3  !
<Estimation Ingham>!
aC3H4+R1H(+M)=C3H5Y(+M)                        4.0E12      0.0
2.7E3      !<WAGnER72>!
                    LOW   /5.6E33       -5.0   4.44E3/
           !<Marinov97> !
aC3H4+R1H(+M)=tC3H5(+M)                  8.5E12      0.0          2.0E3  !
<WAGnER72>!
                    LOW   /1.1E34     -5.0     4.44E3/
           !<Marinov97!
C2H4Z+B4CH=aC3H4+R1H                     1.3E14      0.0         -0.3E3  !
<BAULCH94base>!
R10C2H3V+B5CH2=aC3H4+R1H                 3.0E13      0.0          0.0    !
<MILLER92>!
iC4H3+B5CH2=aC3H4+R9C2H                  2.0E13      0.0          0.0    !
<MILLER92>!
aC3H4+B1O=R1H+B2CO+R10C2H3V              6.6E12      0.0          3.0E3  !
<Aleksandrev nist>!
aC3H4+R2OH=CH2COZ+R4CH3                  2.0E12      0.0         -0.2E3  !
<LIU88>!
aC3H4+R2OH=HCHO+R10C2H3V                 2.0E12      0.0         -0.2E3  !
<LIU88>!
```

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aC3H4+R1H=C3H3+H2                       1.3E6       2.53        9.2E3  !
<est.butatiene>!
aC3H4+B1O=C3H3+R2OH                     6.2E12      0.0         1.9E3  !
<fromAleksandrev nist>!
!d'aprиs leur vitesse de rЙaction total et d'addition !
aC3H4+R2OH=C3H3+H2O                     6.2E6       2.0         0.4E3  !
<est.butadiene>!
aC3H4+R4CH3=C3H3+CH4                    2.0E12      0.0         7.7E3  !
<WU87>!
aC3H4+R9C2H=C3H3+C2H2                   1.0E13      0.0         0.0    !
<WU87>!
aC3H4+C3H5Y=C3H3+C3H6Y                  2.0E12      0.0         7.7E3  !
<DAGAUT92>
aC3H4+R7CH3O=CH3OH+C3H3                       4.0E12      0.0
9.6E3      !<correlations a partir de Heyberger>!
aC3H4+R11C2H5=C2H6+C3H3                    5.0E14      0.0        19.8E3
      !<asbutadiene>!
aC3H4+R10C2H3V=C2H4Z+C3H3             5.0E14      0.0        19.8E3   !
<asbutadiene>!
!aC3H4+R4CH3=C4H7T                      5.7E10      0.0         6.8E3  !
<Scherzer>!
!aC3H4+R4CH3=C4H7T                      3.4E11      0.0         7.4E3
      !<Tsang91x2>!
!aC3H4+R4CH3=iC4H7                      1.6E11      0.0         5.0E3
      !<Tsang73>!
!aC3H4+R4CH3=C4H7T                           0.8E11      0.0
7.4E3      !<Tsang91x2/4>!
aC3H4+R4CH3=iC4H7                       0.4E11      0.0         5.0E3
      !<Tsang73/3>!


!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K
(Tsang91)!
!aC3H4+C3H3=C6H6#+R1H                  1.4E12       0.0        10.0E3  !
<HIDAKA89>!


!******** REACTIONS DE cC3H4 ***** cyclopropene *********!

cC3H4=aC3H4                             1.5E14      0.0    50.5E3  !
<Karni>
cC3H4=pC3H4                             7.1E13      0.0    47.8E3  !
<Karni>
cC3H4+R1H=cC3H3+H2                      5.4E4       2.5    -1.9E3  !
<Heyberger>!
cC3H4+R2OH=cC3H3+H2O                    3.0E6       2.0    -1.5E3  !
<Heyberger>!
cC3H4+R2OH=C2H4Z+R5CHO                  2.8E12      0.0    -1.0E3  !
<Heyberger>!
cC3H3+R3OOH=R2OH+C2H2+R5CHO             1.0E15     -0.8     0.0    !
<Heyberger>!
cC3H3+R4CH3=cC4H6                       1.0E13      0.0     0.0    !
<estimation>!
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cC3H3+R1H=cC3H4                          1.0E14      0.0     0.0    !
<estimation>!

!****** REACTIONS DE C3H5Y ***** (CH2CHCH2(.)) Allyl *****stablilise par
resonnance !

!C3H5Y+R1H=C3H6Y                         2.0E13      0.0         0.0  !
<TSAnG91>!
C3H5Y+R1H=aC3H4+H2                       1.8E13      0.0         0.0  !
TSANG 91!*
C3H5Y+R1H=C3H6Y                          1.0E14      0.0         0.0  !
<allara>!!


!rйaction importante pour la formation de propиne!
C3H5Y+R4CH3=aC3H4+CH4                    3.0E12     -0.32     -0.1E3    !
<TSAnG91>!
C3H5Y+R4CH3=C4H8Y                        1.0E14     -0.32     -0.1E3    !
<TSAnG91>!
C3H5Y+R2OH=aC3H4+H2O                     6.03E12     0.0         0.0  !
Tsang 91!
!peu d'effet de fall off!
C3H5Y+R10C2H3V=aC3H4+C2H4Z               2.4E12      0.0         0.0  !
<TSAnG91>!
!C3H5Y+R11C2H5=aC3H4+C2H6                9.6E11      0.0       -0.1E3    !
<TSAnG91>!
C3H5Y+R11C2H5=aC3H4+C2H6                 2.0E13      0.0       -0.1E3    !
<TSAnG91>MODIF!!!!!
C3H5Y+B1O=R10C2H3V+HCHO                  1.8E14      0.0         0.0  !
<SLAGLE90,LEUnG95>!
!processus non elementaire impliquant la formation-decomposition de
l'hydroperoxyde
!C3H5Y+C3H3=C6H6#+2R1H                   5.6E20     -2.535      1.7E3    !
<MARInOV97>!
C3H5Y+C3H5Y=aC3H4+C3H6Y                  8.4E10      0.0       -0.3E3    !
<TSAnG91>!


!****** REACTIONS DE sC3H5 ***** (CH3CHCH(.)) 2-methyl vinyl *****!

sC3H5=C3H5Y                             5.0E13      0.0        37.0E3 !
<WEISSMAn89>!
R4CH3+C2H2=sC3H5                        6.0E11      0.0       7.7E3 !
<BAULCH94>!

!****** REACTIONS DE tC3H5 ***** (CH3C(.)CH2) 1-methyl vinyl *****!

tC3H5+R1H=aC3H4+H2                       3.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5+R4CH3=aC3H4+CH4                    1.0E11      0.0         0.0   !
<DAGAUT90>!
tC3H5+R10C2H3V=aC3H4+C2H4Z               1.0E12      0.0         0.0   !
<LEUnG95>!
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tC3H5+R11C2H5=aC3H4+C2H6                1.0E12      0.0         0.0   !
<LEUnG95>!
tC3H5+B1O=CH2COZ+R4CH3                  1.8E14      0.0         0.0   !
<LEUnG95>!
tC3H5+O2=R4CH3+B2CO+HCHO                4.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5=C3H5Y                             2.0E13      0.0        47.0E3 !
<Weissman89>!


!****** REACTIONS DE C3H6Y ***** (CH3CHCH2) propene *****!

C2H4Z+B6CH2=C3H6Y                       9.6E13      0.0         0.0  !
<BAULCH94>!
C2H4Z+B5CH2=C3H6Y                       3.2E12      0.0       5.1E3  !
<BAULCH94>!
!duplicate R10C2H3V+R4CH3=C3H6Y         2.5E13      0.0         0.0  !
<TSAnG86>!
C2H4Z+R4CH3=C3H6Y+R1H                   6.6E11      0.0      15.9E3  !
<TSAnG86>!
R11C2H5+B6CH2=C3H6Y+R1H                 9.0E12      0.0         0.0  !
<TSAnG86>!
C2H6+B4CH=C3H6Y+R1H                     1.1E14      0.0      -0.3E3  !
<BAULCH94>!
C3H6Y+R1H=sC3H5+H2                      7.83E5      2.5     12.28E3  !
<TSAnG92>!
C3H6Y+R1H=tC3H5+H2                      3.9E5       2.5      5.82E3  !
<TSAnG92>!
C3H6Y+R1H=C3H5Y+H2                      1.7E5       2.5       2.5E3  !
<TSAnG91>!
C3H6Y+R4CH3=C3H5Y+CH4                   2.2E0       3.5       5.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=sC3H5+CH4                   8.4E-1      3.5      11.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=tC3H5+CH4                   1.3E0       3.5      12.9E3  !
<TSAnG91>!
C3H6Y+R11C2H5=C3H5Y+C2H6                2.2E0       3.5       6.6E3  !
<TSAnG91>!
!C3H6Y+B1O=>CH2COZ+R1H+R4CH3             1.2E+5      2.56    -1130.0  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+B1O=C3H5Y+R2OH                    1.7E11      0.7       5.9E3  !
<TSAnG91>!
!C3H6Y+R2OH=HCHO+R11C2H5                 1.45E12     0.0      -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
!C3H6Y+R2OH=R4CH3+CH3CHO                1.45E12     0.0      -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+R2OH=C3H5Y+H2O                    3.1E6       2.0      -0.3E3  !
<TSAnG91>!
C3H6Y+R2OH=sC3H5+H2O                    1.1E6       2.0      1.45E3  !
<TSAnG91>!
C3H6Y+R2OH=tC3H5+H2O                    2.1E6       2.0       2.8E3  !
<TSAnG91>!
C3H6Y+O2=C3H5Y+R3OOH                    1.9E12      0.0      39.0E3  !
<WALKER93>!
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C3H6Y+R3OOH=C3H5Y+H2O2                  9.6E3       2.6     13.9E3  !
<TSAnG91>!

C3H6Y+R9C2H=pC3H4+R10C2H3V             1.2E13       0.0     0.0     !TSANG
91 mehdi!

!****** REACTIONS DE cC3H6 ***** cyclopropane *****!

cC3H6=C3H6Y                          4.6E14      0.0    62.6E3  !
<Hidaka87>!
cC3H6+R1H=C3H5Y+H2                    1.6E14      0.0   11.7E3   !
<Marshall86>!
cC3H6+R2OH=C3H5Y+H2O                      7.0E7       1.5    1.0E3   !
<Dobe82>!
cC3H6+R4CH3=C3H5Y+CH4                    2.0E11      0.0    9.6E3   !
<Exgas>!

!****** REACTIONS DE R19C3H7 et iC3H7 ***** CH3CH2CH2(.) et  CH3CH(.)CH3
***** !

!R19C3H7 = R4CH3+C2H4Z                       6.400E+12   0.00    31000.0!!
ds мйса PRF
!R19C3H7 = R1H+C3H6Y                         3.000E+13   0.00   38000.00!!
ds мйса PRF
iC3H7 = R1H+C3H6Y                          6.000E+13   0.00   39000.00
R19C3H7 = iC3H7                              1.960E+10   1.00   38600.00
!R19C3H7+O2 =R3OOH+C3H6Y                      1.600E+12   0.00    5000.00
R19C3H7+O2 =R3OOH+C3H6Y                      3.7e16   -1.63    3420 !
2003DES/KLI4415-4427
iC3H7+O2 = R3OOH+C3H6Y                     1.400E+12   0.00    5000.00

!****** Propane (C3H8) chemistry ******!

R11C2H5+R4CH3=C3H8         3.4E13      0.          0.  !(59,-
59)<BAULCH94>!
C3H8+O2=>R3OOH+iC3H7        1.4E+0013  0.000  50323.7  ! BI 2 CN
C3H8+O2=>R3OOH+R19C3H7        4.2E+0013  0.000  53033.0  ! BI 3 CN
B1O+C3H8=>R2OH+iC3H7        2.6E+0013  0.000   5200.0  ! ME 15 CW
B1O+C3H8=>R2OH+R19C3H7        1.0E+0014  0.000   7850.0  ! ME 16 CW
C3H8+R1H=>H2+iC3H7          9.0E+0006  2.000   5000.0  ! ME 17 CW
!C3H8+R1H=>H2+R19C3H7          5.7E+0007  2.000   7700.0  ! ME 18 CW!!ds
мйса PRF
C3H8+R2OH=>H2O+iC3H7       2.6E+0006  2.000   -765.0  ! ME 19 CW
!C3H8+R2OH=>H2O+R19C3H7         5.4E+0006  2.000    450.0  ! ME 20 CW!!ds
мйса PRF
C3H8+R3OOH=>H2O2+iC3H7     4.0E+0011  0.000  15500.0  ! ME 21 CN
!C3H8+R3OOH=>H2O2+R19C3H7       1.2E+0012  0.000  17000.0  ! ME 22 CN!!ds
мйса PRF
C3H8+R4CH3=>CH4+iC3H7      2.0E+0011  0.000   9600.0  ! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7        6.0E-0001  4.000   8200.0  ! ME 24 CN!!ds
мйса PRF
C3H8+R5CHO=>HCHO+iC3H7     1.0E+0007  1.900  17000.0  ! ME 25 CN
C3H8+R5CHO=>HCHO+R19C3H7        2.0E+0005  2.500  18500.0  ! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7    2.0E+0011  0.000  11000.0  ! ME 33 CN
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!C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! ME 34 CR!!ds
мйса PRF
C3H8+iC3H7=>C3H8+R19C3H7        8.4E-0003  4.200   8700.0  ! ME 35 CN
R1H+iC3H7=>C3H8             8.3E+0012  0.000      0.0  ! CO 36 K

!****************Reactions of Acetone*************************!
!R14CH3CO+R4CH3=>C2H6CO                    4.0E15     -0.8        0. !
(231,-231)<TSAnG86>!
R14CH3CO+R4CH3=>C2H6CO                    2.7E15     -0.8        0. !
(231,-231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low
pressure.
iC3H7+B1O=>C2H6CO+R1H                 1.0          0.0         0.0     !
Tsang88 (Nist)
C2H6CO+O2=>R3OOH+CH2COZ+R4CH3         4.2E12       0.0         49.28E3 !
Kingas!
C2H6CO+B1O=>CH2COZ+R4CH3+R2OH         1.02E14      0.0         7.85E3  !
Buda!
C2H6CO+R1H=>CH2COZ+R4CH3+H2           5.70E07      2.0         7.70E3

C2H6CO+R2OH=>CH2COZ+R4CH3+H2O         5.34E06      2.0         0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4        6.00E-1      4.0         8.20E3

C2H6CO+R3OOH=>CH2COZ+R4CH3+H2O2       1.20E12      0.0         17.0E3

!*****************Reactions of Propanal************************!

!R5CHO+R11C2H5=>C2H5CHO                    1.8E13       0.          0.
!(141,-141)<TSAnG86>!
!C2H5CHO=R5CHO+R11C2H5                     1.07E+14     0.0       62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240
R5CHO+R11C2H5=C2H5CHO                     3.4E+13      0.0       0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R5CHO+R11C2H5                     2.45E+15     0.0       72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)
R13CH2CHO+R4CH3=C2H5CHO                   3.4E+13      0.0       0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R4CH3+R13CH2CHO                   7.00E+15     0          81703
!Baulch et al 1992,J. Phys.Chem.Ref.Data 21 411–429.
B1O+C3H6Y=>C2H5CHO                        1.000E+12    0          5000.0
!Mech Franssoldati
!C2H5CHO+R1H=H2+B2CO+R11C2H5               4.0E13       0.0        4.2E3
!<Heyberger>! ADZ 714
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5             4.0E12       0.0        0.5E3
!<Heyberger>! ADZ 715

!C2H5CHO=R4CH3+R13CH2CHO                   2.00E+16     0          83800.
!Mech Franssoldati
C2H5CHO+R1H=H2+R25C2H5CO                  1.17E+11     0.0        6000
!Decottignies et al.2002.
C2H5CHO+B1O=R2OH+R25C2H5CO                5.000e+12    0.0
1.790e+03  !Curran et al. Fuel (2011) 90(1) 331–338.
C2H5CHO+R2OH=H2O+R25C2H5CO                2.690e+10    0.760
-3.400e+02  !Curran et al. Fuel (2011) 90(1) 331–338.
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R25C2H5CO=B2CO+R11C2H5                      2.95E+12     0.0       11100.0
!Decottignies et al.2002.

!*************************************************

!*************************************************


!*************************************************!
!     REACTIONS DES ESPECES NON OXYGENES EN C4      !
!*************************************************!

!****** REACTIONS DE C4H2  ***** (CH///CC///CH) diacetylene ***** !

R9C2H+R9C2H=C4H2                        1.8E13       0.0         0.0   !
<TSAnG86>!
2C2H2=C4H2+H2                           1.5E13       0.0      42.7E3     !
<LEUnG95>!
C2H2+R9C2H=C4H2+R1H                     9.0E13       0.0         0.0   !
BAULCH94!
!C4H2+R1H=C2H2+R9C2H                    6.0E14       0.0      15.4E3     !
<MEREDITH86>!
C4H2+R2OH=>R5CHO+C3H2                    6.7E12       0.0      -0.4E3    !
<LEEDS-website>!
C4H2+O2=R12CHCOZ+R12CHCOZ               9.6E12       0.0      31.1E3     !
<HIDAKA02>!!!
C4H2+R9C2H=>C6H2+R1H                    4.0E13       0.0         0.0   !
<MEREDITH86>!
C6H2+R1H=>C4H2+R9C2H                    9.3E14       0.0      15.1E3     !
<MEREDITH86>!

!****** REACTIONS DE nC4H3  ***** (ĽCH//CHC///CH) **********!

nC4H3(+M)=C4H2+R1H(+M)                  1.0E14       0.0      36.0E3     !
<MILLER92>!
          LOW   /1.0E14 0.0 30E3/
          TROE / 1.0  1.0  1.0E8/
C3H3+B4CH=nC4H3+R1H                     7.0E13       0.0         0.0   !
<MILLER92>!
!C3H3+B4CH=nC4H3+R1H                    5.0E13       0.0         0.0   !
<MILLER92>!
R9C2H+R10C2H3V=nC4H3+R1H                1.8E13       0.0         0.0   !
<TSAnG86>!
nC4H3+R1H=iC4H3+R1H                     2.4E11       0.79     2.41E3     !
<WAnG97>20Torr!
nC4H3+R1H=C4H2+H2                       0.6E13       0.0         0.0   !
<0.5*la cst de la react(c2h3+h)>!
2C2H2=nC4H3+R1H                         1.0E12       0.0      64.1E3   !
<LEUnG95>!
nC4H3+R2OH=C4H2+H2O                     1.5E13       0.0         0.0   !
<0.5* la cst de la react(c2h3+oh)>!
!***
!nC4H3+C2H2=C6H4#+R1H                    1.64E9       0.73     12.2E3   !
<WESTMORELAnD89, p=2.6kPa>!
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nC4H3+C2H2=C6H4#+R1H                3.0E-11      6.48      6.6E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H4+R1H                 29.6         3.33      9.6E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H4+R1H                2.77E-7      5.59      6.0E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H5                     1.73E11     -0.41      4.0E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H5                    6.17E15     -1.51      4.8E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=C6H5#                     3.33E24     -3.89      9.2E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=C6H5#                    7.0E14      -0.86      6.4E3      !
<WESTMORELAnD89, p=101kPa>!
!***


!****** REACTIONS DE iC4H3  ***** (CH2//CĽC///CH) *****

iC4H3=nC4H3                          1.5E13       0.0      67.8E3   !
<LEUnG95>!
iC4H3(+M)=C4H2+R1H(+M)               1.0E14       0.0      55.0E3     !
<MILLER92>!
           LOW  /2.0E15 0.0 48E3/
           TROE /1.0  1.0  1.0E8/
C3H2+B5CH2=iC4H3+R1H                 1.2E14       0.0       0.8E3     !
as(7)<BAULCH94>!
iC4H3+R1H=2C2H2                      2.40E19      -1.6       2800   !
<WAnG97>20Torr! !
C3H3+B4CH=iC4H3+R1H                  7.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R1H=C4H2+H2                    1.2E13       0.0         0.0   !
<equiv a la cst de la react(c2h3+h)>!
iC4H3+B1O=CH2COZ+R9C2H               2.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R2OH=C4H2+H2O                  3.0E13       0.0         0.0   !<
equiv a la cst de la react(c2h3+oh)>!
iC4H3+O2=CH2COZ+R12CHCOZ             1.0E12       0.0         0.0   !
<MILLER92>!
*
iC4H3+R10C2H3V=2C3H3                 4.0E12       0.0         0.0   !
MILLER 92 !
iC4H3+R10C2H3V=>lC6H5+R1H             6.0E12       0.0         0.0   !
MILLER 92!

!****** REACTIONS DE C4H4  ***** (CH2//CHC///CH) vinylacetylene *****!

C3H3+B5CH2=C4H4+R1H                  4.0E13       0.0           0.0 !
<MILLER92>!
R10C2H3V+C2H2=>C4H4+R1H              2.0E13       0.0        25.1E3 !
(40,-40)<DOUTE95>!
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C4H4+R1H=>R10C2H3V+C2H2                 2.0E13       0.0        12.4E3 !
<DOUTE95>
C2H4Z+R9C2H=C4H4+R1H                    1.2E13       0.0           0.0 !
(50,-50)<TSAnG86>!
C4H4+R1H=nC4H3+H2                       2.0E7        2.0         15.E3 !
<Miller 92>!
C4H4+R1H=iC4H3+H2                       3.0E7        2.0          5.E3 !
<Miller 92>!
R9C2H+C4H4=>C2H2+iC4H3                  4.0E13       0.0           0.0 !
<MEREDITH86>!
C2H2+iC4H3=>R9C2H+C4H4                  3.0E13       0.0        27.9E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+nC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
nC4H3+C2H4Z=>R10C2H3V+C4H4              3.5E11       0.0        13.4E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+iC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
iC4H3+C2H4Z=>R10C2H3V+C4H4              1.3E11       0.0        24.1E3 !
<MEREDITH86>!
C4H4+C2H2=C6H5#+R1H                     1.0E09       0.0       30.02E3 !
BENSON  !MF
C4H4+R10C2H3V=C6H6#+R1H                 1.9E12       0.0         2.5E3 !
<LInSTEDT96>!
C4H4+B1O=aC3H4+B2CO                     3.0E13       0.0         1.8E3 !
<LEUnG95>!
C4H4+B1O=pC3H4+B2CO                     2.7E13       0.0         1.8E3 !
<MILLER>!
C4H4+R2OH=nC4H3+H2O                     7.5E6        2.0         5.0E3 !
<MILLER92>!
C4H4+R2OH=iC4H3+H2O                     1.0E7        2.0         2.0E3 !
<MILLER92>!
aC3H4+aC3H4=C2H4Z+C4H4                  1.0E15       0.0        48.0E3 !
<HIDAKA89>!


!****** REACTIONS DE tC4H4  ***** (CH2//C//C//CH2) *****!

tC4H4+R2OH=iC4H3+H2O                    2.0E7        2.0         2.0E3   !
<Marinov>!
tC4H4+R1H=iC4H3+H2                      3.0E7        2.0         6.0E3   !
<Marinov>!

!****** REACTIONS DE nC4H5  ***** (ĽCH//CHCH//CH2) *****

nC4H5(+M)=R1H+C4H4(+M)                  1.0E14       0.0       37.0E3      !
<MILLER92>!
            LOW   /1.00e+14 0.0 30000/
nC4H5+R1H=C4H4+H2                       1.5E13       0.0           0.0    !
<WAnG97>!
nC4H5+R1H=iC4H5+R1H                     1.0E14       0.0           0.0    !
<MILLER92>!
nC4H5+R4CH3=C5H8                        1.0E13       0.0           0.0    !
<estimated> !
```

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nC4H5=C2H2+R10C2H3V                    1.0E14       0.0       43.9E3      !
<HIDAKA96>!
!***
!MF car lC6H6 n'intervient qu'ici
!nC4H5+C2H2=lC6H6+R1H                   1.17E-15     7.84       2.0E3  !
<WESTMORELAnD89, p=2.6kPa>!
!nC4H5+C2H2=lC6H6+R1H                  3.47E-15     7.73       2.5E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H6#+R1H                   1.90E7       1.47       4.2E3  !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H6#+R1H                  2.38E8       1.18       3.7E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=lC6H7                       8.74E12     -1.27       3.6E3 !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=lC6H7                      7.24E14     -1.38       4.0E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H7#                       1.96E19     -3.35       5.2E3 !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H7#                      7.12E21     -3.64       6.3E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H7+R1H               8.28E-28    11.89       5.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H7+R1H              3.55E-43    16.16      -0.2E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H8                   2.90E15     -0.78       1.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H8                  1.50E13     -0.075      0.1E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H8#                   5.50E15     -1.67       1.5E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H8#                  8.53E13     -1.11       0.8E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H6#+H2                2.80E-7      5.63      -1.9E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H6#+H2               1.84E-13     7.07      -3.6E3 !
<WESTMORELAnD89, p=101kPa>!
!***
nC4H5+R2OH=C4H4+H2O                    2.5E12       0.0          0.0  !
<WAnG97>!

!nC4H5+O2=R5CHO+C2H3CHO                 1.7e29      -5.31       6.5E3 !MF
as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>
nC4H5+O2=R5CHO+C2H3CHO                5.67E28      -5.31       6.5E3 !MF
nC4H5+O2=C2H4Z+B2CO+R5CHO             1.13e29      -5.31       6.5E3 !MF
nC4H5+O2=C4H4+R3OOH                   5.19E15       -1.26        3.31e3  !
MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>
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 !****** REACTIONS DE iC4H5  ***** (CH2//CHCґ//CH2) *****stablilise par
resonnance
iC4H5=nC4H5                          1.5E13       0.0        67.8E3 !
<LEUnG95>!


iC4H5(+M)=R1H+C4H4(+M)               1.0E14       0.0        50.0E3 !
<MILLER92>!
            LOW   /2.0E15 0.0 42000/
iC4H5+R1H=C4H4+H2                    3.0E13       0.0           0.0  !
<WAnG97>!
iC4H5+R4CH3=iC5H8                    1.0E13       0.0           0.0  !
<estimated> !
2R10C2H3V=iC4H5+R1H                  1.5E30      -4.95       13.0E3  !
<WAnG97>20Torr!
!***2R10C2H3V=iC4H5+R1H              1.2E22      -2.44       13.7E3  !
<WAnG97>760Torr!
iC4H5+R2OH=C4H4+H2O                  5.50E12      0.0           0.0  !
<WAnG97>!
iC4H5+O2=HCHO+CH2CHCO                4.5E16      -1.39         1.0E3  !
estimй par{O2+C2H3=HCHO+CHO}!
iC4H5+O2=C4H4+R3OOH                  1.34E6       1.61          -400  !
estimй par {O2+C2H3=C2H2+OOH}!


!****** REACTIONS DE C4H5-1s  ***** (CH3/CHґ/C///CH) *****stablilise par
resonnance

!C4H5-1s=R1H+C4H4                      3.0E13       0.0        45.0E3 !
<HIDAKA96>!
C4H5-1s=R1H+C4H4                       6.0E13       0.0        50.4E3 !
add inverse!
! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-1s+R1H=C4H4+H2                    2.0E13       0.0         0.0   !
<MILLER92/BRAUn89>!
C4H5-1s+B1O=R9C2H+CH3CHO               1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
C4H5-1s+R2OH=C4H4+H2O                  2.0E13       0.0         0.0   !
<MILLER92>!
C4H5-1s+R2OH=R5CHO+sC3H5               4.0E13       0.0         0.0   !
<WAnG97>!
C4H5-1s+O2=R5CHO+B2CO+C2H4Z            3.0E10       0.0         2.9E3 !
<MILLER92/SLAGUE88>!
C4H5-1s+C4H5-1s=C8H10#                 1.0E12       0.0         0.0   !
<STEIn90>shocktube!

!****** REACTIONS DE C4H5-1p  ***** (CH2ґ/CH2/C///CH) *****

!C4H5-1p=R1H+C4H4                       3.0E13       0.0        45.0E3 !
<HIDAKA96>!
!C4H5-1p=R1H+C4H4                       4.0E13       0.0        38.8E3 !
<HIDAKA96>!
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```
C4H5-1p=R9C2H+C2H4Z                        2.0E14       0.0        57.0E3 !
<HIDAKA96>!
C4H5-1p+O2=C4H4+R3OOH                      1.6E12       0.0         5.0E3 !
PAG00!
C4H5-1p=C4H5-1s                            5.0E12       0.0        37.4E3 !
PAG00!

!****** REACTIONS DE C4H5-2  ***** (CH3/C///C/CH2Ґ) *****stablilise par
resonnance

!C4H5-2=R1H+tC4H4                          3.0E13       0.0        50.0E3 !
<fromHIDAKA96+5!
C4H5-2=R1H+tC4H4                           6.0E13       0.0        54.3E3 !
toto!

!C4H5-2=iC4H5                              3.0E13       0.0        50.0E3 !
<fromHIDAKA96>!
C4H5-2=iC4H5                               5.0E12       0.0        50.5E3 !
PAG00!
C4H5-2+C4H5-2=C8H10#                       1.0E12       0.0           0.0 !
<STEIn90>shocktube!

! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-2+B1O=C3H3+HCHO                     1.4E14       0.0          0.0   !
<MILLER92/SLAGUE91>!
C4H5-2+R2OH=R10C2H3V+B2CO+R4CH3          4.0E13       0.0          0.0   !
<WAnG97>!
C4H5-2+O2=CH2COZ+B2CO+R4CH3              3.0E10       0.0          2.9E3 !
<MILLER92/SLAGUE88>!


!****** REACTIONS DE C4H6Z2  ***** 1,3 Butadiene (CH2CHCHCH2) *****!
!R10C2H3V+R10C2H3V=C4H6Z2                6.8E12       0.0          0.0   !
<TSAnG86 P=2.6KPa T=1500>!
!R10C2H3V+R10C2H3V=C4H6Z2                9.8E14      -0.5          0.0   !
<HIDAKA96shocktube>!
!
!C4H6Z2=C4H4+H2                           2.5E15       0.0       94.7E3   !
<HIDAKA96>
!C4H6Z2=iC4H5+R1H                         1.4E15       0.0       98.0E3   !
<HIDAKA96>!
!
!C2H4Z+R10C2H3V=C4H6Z2+R1H                5.0E11       0.0        7.3E3   !
<TSAnG86>!
!
!C4H6Z2+R1H=nC4H5+H2                        1.3E6        2.53      12.2E3   !
<WAnG97>!
!C4H6Z2+R1H=iC4H5+H2                        6.6E5        2.53       9.2E3   !
<WAnG97>!
!
!C4H6Z2+R1H=C4H7-1                  2.6E13       0          3.2E3   !
ESTIMATED *2!
!C4H6Z2+R1H=C4H7Y                   2.6E13       0         1.56E3   !
ESTIMATED *2!
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!C4H6Z2+R1H=C4H7-1                    1.3E13       0         3.2E3   !
ESTIMATED
!C4H6Z2+R1H=C4H7Y                     1.3E13       0        1.56E3   !
ESTIMATED !
!
!C4H6Z2+R4CH3=nC4H5+CH4                7.0E13       0.0      18.5E3   !
<WU87>!
!C4H6Z2+R4CH3=iC4H5+CH4                7.0E13       0.0      15.5E3   !
<WU87-3kcal>!
!C4H6Z2+R4CH3=C5H9Y              6.3E10       0.0      7.49E3   ! PERRIN
88 nist!
!C4H6Z2+R4CH3=iC5H9              1.8E11       0.0       8.0E3   !
Estimated*2!
!C4H6Z2+R4CH3=C5H9Y                   6.31E10      0.0      7.49E3   !
PERRIN 88 nist!
!C4H6Z2+R4CH3=iC5H9                   9.64E10      0.0       8.0E3   !
Estimated!
!
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z           5.0E14       0.0      22.8E3   !
<HIDAKA96>!
!C4H6Z2+R10C2H3V=iC4H5+C2H4Z           5.0E14       0.0      19.8E3   !
<HIDAKA96-3kcal>!
!
!C4H6Z2+B1O=C3H5Y+R1H+B2CO             6.0E08       1.45      0.9E3   !
<LEUnG95,BREZInSKY84>!
!
!R10C2H3V+C4H6Z2=C6H8#+R1H             7.4E014     -0.66     8.42E3   !
<frenklach >!
!R10C2H3V+C4H6Z2=C6H8#+R1H             2.28E12     -0.24      9.9E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H8#+R1H             4.15E-11     6.39      2.4E3   !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+C4H6Z2=lC6H8+R1H             1.0E10       1.05     14.0E3    !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H8+R1H              2.48E-15     8.20      6.3E3    !
<WESTMORELAnD89, p=101kPa>!
!***
!C4H6Z2+C2H2=C6H8#                      2.3E12       0.0      35.0E3    !
<WESTMORELAnD89>!
!***
!MF car lC6H9 n'intervient qu'ici
!R10C2H3V+C4H6Z2=lC6H9                 5.48E28     -5.31      9.3E3    !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H9                  1.48E12     -0.17      3.2E3    !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+C4H6Z2=C6H9Z#                1.64E29     -6.12      9.6E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H9Z#                 7.06E13     -1.35      4.0E3   !
<WESTMORELAnD89, p=101kPa>!
!***
!C4H6Z2+C2H4Z=C6H10#                    2.3E10       0.0      27.0E3   !
<WESTMORELAnD89>!
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```
!C4H6Z2+R2OH=nC4H5+H2O                6.2E6        2.0        3.4E3    !
<WAnG97>!
!C4H6Z2+R2OH=iC4H5+H2O                3.1E6        2.0        0.4E3    !
<WAnG97>!
!C4H6Z2+R2OH=C3H5Y+HCHO               2.8E12       0.0       -0.9E3    !
<LInSTEDT96>!
!C4H6Z2+R2OH=CH3CHO+R10C2H3V          5.6E12       0.0       -0.9E3    !
<fromLInSTEDT96>!
!C4H6Z2+O2=iC4H5+R3OOH                4.0E13       0.0       57.9E3    !
<LEUnG95>!
!C4H6Z2+C3H3=nC4H5+aC3H4              1.0E13       0.0       22.5E3    !
<HIDAKA96>!
!C4H6Z2+C3H3=iC4H5+aC3H4              1.0E13       0.0       19.5E3    !
<HIDAKA96-3kcal>!

!****** REACTIONS DE C4H6-12  ***** (1,2) Butadiene (CH2CCHCH3) *****

!C4H6-12=C4H6Z2                       3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-12=iC4H5+R1H                    4.2E15       0.0        92.6E3 !
<LEUnG95>!
!C4H6-12+R1H=R10C2H3V+C2H4Z           4.0E11       0.0           0.0 !
<LEUnG95>!
!C4H6-12=C3H3+R4CH3                   7.3E14       0.0        75.4E3 !
<kingas1500K>!
!C4H6-12+R1H=C4H7-2                   1.3E13       0.0         1.6E3 !
<heyberger> !
!C4H6-12+R1H=C4H7Y                    1.2E11       0.69        3.0E3 !
<heyberger>!
!C4H6-12+R1H=C4H7T                    1.3E13       0.0         3.2E3 !
<heyberger> !
!C4H6-12+R1H=iC4H5+H2                 1.7E5        2.5         2.5E3 !
<asTSAnG91>!
!C4H6-12+R4CH3=iC4H5+CH4              2.2E0        3.5         5.7E3 !
<asTSAnG91>!
!C4H6-12+R11C2H5=iC4H5+C2H6           2.2E0        3.5         6.6E3 !
<asTSAnG91>!
!C4H6-12+B1O=iC4H5+R2OH               1.7E11       0.7         5.9E3 !
<asTSAnG91>!
!C4H6-12+R2OH=iC4H5+H2O               3.1E6        2.0        -0.3E3 !
<asTSAnG91>!
!C4H6-12+R3OOH=iC4H5+H2O2             9.6E3        2.6        13.9E3 !
<asTSAnG91>!


!****** REACTIONS DE (c-C4H6)  ***** methyl-cyclopropene  *****

!B6CH2+pC3H4=cC4H6                    1.8E14       0.0         0.0   !
<LEUnG95>!
!cC4H6=C4H6Z2                         3.0E13       0.0        42.3E3 !
<LEUnG95>!
!cC4H6=C4H6-12                        3.0E13       0.0        43.8E3 !
<LEUnG95>!
```

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!****** REACTIONS DE (C4H6-1) *****  1 Butyne *****

!C4H6-1=C4H6-12                          2.5E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-1=C4H5-1s+R1H                      7.7E14       0.0        87.9E3 !
Kinga&dH Melius!
!C4H6-1=C4H5-1p+R1H                      9.1E14       0.0        99.6E3 !
Kingas!
!C4H6-1=>C3H3+R4CH3                     3.0E15       0.0        75.8E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                 1.3E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R11C2H5+C2H2                6.5E4        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                  3.2E12       0.0         1.7E3 !
<asWAGnER72>!
!C4H6-1+R1H=R11C2H5+C2H2                 3.2E12       0.0         1.7E3 !
<asWAGnER72>!
! Les rйactions suivantes sont deduites de celles de 1-C4H8 generes par
EXGAS
!C4H6-1+R1H=H2+C4H5-1s                   5.4E4        2.5        -1.9E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1s                1.5E12       0.0         7.1E3 !
<EXGAS>!
!C4H6-1+B1O=R2OH+C4H5-1s                 8.8E10       0.7         3.2E3 !
<EXGAS>!
!C4H6-1+R2OH=H2O+C4H5-1s                 3.0E6        2.0        -1.5E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1s               1.4E12       0.0        36.0E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s                1.4E12       0.0        41.4E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s               4.2E12       0.0        49.5E3 !
<DAGAUT90sec>!
!C4H6-1+R3OOH=>H2O2+C4H5-1s              6.4E3        2.6        12.4E3 !
<EXGAS>!
! Les rйactions suivantes sont deduites de celles generes par EXGAS pour
H primaires
!C4H6-1+R1H=H2+C4H5-1p                   2.9E7        2.0         7.7E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1p                3.7          4.0         8.2E3 !
<EXGAS>!MF
!C4H6-1+B1O=R2OH+C4H5-1p                 5.1E13       0.0         7.8E3 !
<EXGAS>!
!C4H6-1+R2OH=>H2O+C4H5-1p                2.7E6        2.0        -0.4E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1p                1.2E13       0.0        49.0E3 !
<EXGAS>!
!C4H6-1+R3OOH=>H2O2+C4H5-1p              6.0E11       0.0        17.0E3 !
<EXGAS>!
! Les rйactions d'addition suivantes sont deduites de celles de pC3H4
!C4H6-1+B1O=R12CHCOZ+R11C2H5             1.5E13       0.0         2.1E3 !
<asWARnATZ84>!
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!C4H6-1+R2OH=CH2COZ+R11C2H5           4.3E11       0.0        -0.8E3 !
<asBOODAGHIAnS87>!

!***** REACTIONS DE (C4H6-2)***** 2 Butyne  *****

!C4H6-2=C4H6Z2                        3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-2=C4H6-12                       3.0E13       0.0        67.0E3 !
<HIDAKA96>!
!C4H6-2=C4H5-2+R1H                    2.0E14       0.0        87.3E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4              2.6E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4               6.5E12       0.0         1.7E3 !
<asWAGnER72>


! Les rйactions suivantes sont deduites de celles de pC3H4
!C4H6-2+R1H=C4H5-2+H2                 3.4E5        2.5          2.5E3 !
<asTSAnG91*2>!
!C4H6-2+R4CH3=C4H5-2+CH4              4.4E0        3.5          5.7E3 !
<asTSAnG91*2>!
!C4H6-2+B1O=B2CO+R10C2H3V+R4CH3       1.5E13       0.0          2.1E3 !
<asWARnATZ84>!
!C4H6-2+B1O=R2OH+C4H5-2               1.2E11       0.7          7.6E3 !
<asTSAnG91*2>!
!C4H6-2+R2OH=B2CO+C2H4Z+R4CH3         4.3E11       0.0         -0.8E3 !
<asBOODAGHIAnS87>!
!C4H6-2+R2OH=C4H5-2+H2O               6.2E6        2.0         -0.3E3 !
<asTSAnG91*2>!
!C4H6-2+O2=C4H5-2+R3OOH               4.2E12       0.0         44.0E3 !
<InGHAM95*2>+4!
!C4H6-2+R3OOH=C4H5-2+H2O2             1.9E4        2.6         13.9E3 !
<asTSAnG91*2>!


!******* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y                         3.34E09       1.0       39.1E3  !
ESTIMATED !
!C4H7-1=C4H7V                         3.3E9         1.0       20.7E3  !
Estimated!
!C4H7-1=C2H4Z+R10C2H3V                2.0E13        0.0       35.5E3  !
Estimated!
!C4H7-1+R4CH3=C5H10                   2.0E13        0.0          0.0  !
Estimated !
!C4H7-1+R1H=C4H8Y                     1.0E14        0.0          0.0  !
Estimated!

!******* Reactions de C4H7Y (CH3-CH.-CH=CH2)!*****stablilise par
resonnance
!C4H7Y+R1H=C4H8Y                      2.0E13        0.0          0.0  !
asTSANG 91!!
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!C4H7Y+R1H=H2+C4H6Z2                    0.9E13        0.0          0.0  !
asTSANG 91!!
!C4H7Y+R1H=H2+C4H6-12                   0.9E13        0.0          0.0  !
asTSANG 91!
!C4H7Y+R3OOH=R2OH+C2H3CHO+R4CH3         1.0E15       -0.8          0.0  !
<Heyberger>!
!C4H7Y+R4CH3=iC5H10                     0.5E13        0.0          0.0  !
Estimated !

!**************Reactions de C4H7V (CH3-CH2-CH=CH.)*******!
!C4H7V=C4H7Y                           1.9E10         1.0       36.3E3  !
Heyberger!
!C4H7V=R11C2H5+C2H2                    2.0E13         0.0       33.0E3  !
Heyberger!

!**************Reactions de C4H7-2 (CH3-C.=CH-CH3)*****!
!C4H7-2=C4H7Y                          2.9E10     1.0         37.8E3  !
ESTIMATED !
!C4H7-2=R4CH3+pC3H4                    2.0E13      0.0      31.5E3  !
ESTIMATED !

!**************Reactions de C4H7T (CH2=C.-CH2-CH3)********!

!C4H7T=C4H7-1                          3.34E09      1.0       40.6E3   !
ESTIMATED !
!C4H7T=C4H7Y                           2.0E13       0.0       47.0E3   !
<Heyberger>!
!C4H7T=R4CH3+aC3H4                     2.0E13       0.0       32.5E3   !
ESTIMATED !

!**************Reactions du 1-butene!

!C4H8Y+O2=C4H7Y+R3OOH                  3.6E12       0.0         38.2E3  !
<Heyberger>!
!C4H8Y+R1H=C4H7Y+H2                    5.4E4        2.5         -1.9E3  !
<Heyberger>!
!C4H8Y+R2OH=>HCHO+R4CH3+C2H4Z          1.4E12       0.0         -1.0E3  !
<Heyberger>!
!C4H8Y+R2OH=R4CH3+C2H5CHO              1.4E12       0.0         -1.0E3  !
<Heyberger>!!ds мйса PRF
!C4H8Y+R2OH=C4H7Y+H2O                  3.0E6        2.0        -1.52E3  !
<Heyberger>!
!C4H8Y+R4CH3=C4H7Y+CH4                 1.0E11       0.0          7.3E3  !
<Heyberger>!

!C2H5CHO+R1H=H2+B2CO+R11C2H5           4.0E13       0.0          4.2E3  !
<Heyberger>!
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5         4.0E12       0.0          0.5E3  !
<Heyberger>!

!***********reactions de iC4H8********!
!iC4H8+R2OH=iC3H7+HCHO                 1.4E12       0.0      -1040.0    !
(idem RF)
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!iC4H8+R1H=>iC4H7+H2                    3.5E5        2.5        2510    !
(idem RF)
!iC4H8+R2OH=>iC4H7+H2O                  6.0D+06    2.000      -298.0    !
MES 878<C.M.>!(idem RF)
!iC4H7+R1H=iC4H8                       1.0E14       0.0         0.0    !
<estimation>!
!iC4H7+R3OOH=>R2OH+HCHO+tC3H5           1.0E15      -0.8         0.0    !
<Heyberger>!


!
**********************************************************************
**!
!
**********************************************************************
*********!
!*              MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE
*!
!*
*!
!*    efficiency  coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
**********************************************************************
*********!
!*           PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
**********************************************************************
*********!


!REACTIONS OF BENZENE MOLECULES!
!***Umimolecular inititiation!
C6H5#+R1H(+M)=C6H6#(+M)              1.0E14      0.0        0.0      !
<WANG97>!
                          LOW   /6.6E75  -16.3   7.0E3/
                          TROE /1.0 0.1 585 6113/
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
!***Bimolecular inititiation!
C6H6#+O2=C6H5#+R3OOH                6.0E13      0.0          63.4E3   !
<ALZUETA00>!
!***additions!
C6H6#+R1H=C6H7#                      3.2E13      0.0         3.2E3   !
<MEBEL97>!
C6H6#+B1O=C6H5O#+R1H                 2.8E13      0.0        4.91E3   !
<EMDEE92>!
C6H6#+R2OH=C6H5OH#+R1H               1.3E13      0.0        10.6E3   !
<BAULCH94>!
C6H6#+R9C2H=C6H5#C2H+R1H             5.0E13      0.0           0.0   !
<WANG97>!
C6H6#+R10C2H3V=styrene+R1H           7.9E11      0.0         6.4E3   !
<WANG97>!
!***Metatheses!
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!*modif Zhenyu*!
!C6H6#+R1H=C6H5#+H2                  6.0E8       1.8         16.8E3   !
<MEBEL97>!
C6H6#+R1H=C6H5#+H2                   1.22E8      2.031      15.88E3   !
calcul CBS-QB3 Fournet

C6H6#+B1O=C6H5#+R2OH              2.0E13    0.0         14.7E3   !
<LINDSTEDT94>!

!*modif Zhenyu*!
!C6H6#+R2OH=C6H5#+H2O                1.6E8       1.42        1.45E3   !
<BAULCH92>!
C6H6#+R2OH=C6H5#+H2O                  1.36E4      2.7       0.6196E3   !as
toluene+R2OH=C6H4CH3+H2O

!*modif Zhenyu*!
!C6H6#+R3OOH=C6H5#+H2O2              5.5E12      0.0         28.9E3   !
<BAULCH94>!
C6H6#+R3OOH=C6H5#+H2O2               9.2E12      0.0        28.81E3   !as
toluene+R3OOH=C6H4CH3+H2O2

!*modif Zhenyu*!
!C6H6#+R4CH3=C6H5#+CH4                2.0E12      0.0         15.0E3   !
<ZHANG89>!
C6H6#+R4CH3=C6H5#+CH4                2.07E0      3.861       13.3E3   !
calcul CBS-QB3 Fournet

C6H6#+R11C2H5=C6H5#+C2H6             6.3E11      0.0         15.0E3   !
<ZHANG89>!
C6H5#+C3H6Y=C6H6#+C3H5Y              7.94E13     0.0        11.94E3   !MF
<Heckmann,Hippler,Troe(1996)>
C6H6#+nC4H5=C6H5#+C4H6Z2             6.3E11      0.0         15.0E3   !
estimated!
C6H6#+iC4H5=C6H5#+C4H6Z2             6.3E11      0.0         20.0E3   !
estimated!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=lC6H7                          2.5E14      0.7        41.8E3    !
<WEISSMAN89!

!***Decomposition by beta-scission!
!C6H7#=>C2H2+nC4H5                   2.0E13      0.0        50.0E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
HEYBERGER02!
!***Oxidation!
C6H7#+O2=C6H6#+R3OOH                 7.9E11      0.0         9.9E3    !
estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combimations!
C6H7#+R1H=C6H8#                      1.0E14      0.0         0.0      !
estimated!
```

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!***Disproportionnations!
C6H7#+R1H=C6H6#+H2                  3.3E12      0.0        0.0      !
<RISTORI01>!
C6H7#+R2OH=C6H6#+H2O                1.0E13      0.0        0.0      !
estimated!
C6H7#+R4CH3=C6H6#+CH4               3.0E12     -0.32      -0.1E3    !
estimated!
C6H7#+C6H7#=C6H6#+C6H8#             8.4E10      0.0       -0.3E3    !
estimated!
!analogy with the disproprotionnations ofC3H5Y proposed by TSANG91!

!REACTIONS OF C6H5# RADICALS!
!***Isomerization!
C6H5#=lC6H5                         5.0E13      0.0       72.5E3    !
<BRAUN89>!
!lC6H5 = ch///c/ch//ch/ch//ch(.)!
lC6H5=>2C2H2+R9C2H                   2.0E13      0.0       51.0E3   !
estimated!
!DH298 =44kcal/mol, Eadd=7 kcal/mol!
lC6H5=lC6H4+R1H                          2.0E12      0.0
41.0E3   !estimated!
!lC6H4 = ch///c/ch//ch/c///ch , DH298 =38kcal/mol, Eadd=3 kcal/mol!
!from BRAUN89 at 1500 K!
!***Reactions with O2!
C6H5#+O2=C6H5O2                     2.2E19     -2.5         0.0    !
estimated!

C6H5#+O2=C6H5O#+B1O                 2.6E13      0.0        6.1E3    !
<FRANK94>!
C6H5#+O2=OC6H4O+R1H                 3.0E13      0.0        9.0E3    !
<FRANK94>!


!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!
!***Additions!
C6H5#+C2H2=C6H5#C2H+R1H             4.0E13      0.0       10.1E3    !
<MARINOV97>!
C6H5#+C6H6#=biphenyl+R1H            5.6E12     -0.074      7.5E3    !
<WANG97>!
!***Combinations!
C6H5#+B1O=C5H5#+B2CO               1.0E14      0.0          0.0     !
<FRANK94>!
C6H5#+R2OH=C6H5OH#                    1.0E13       0.0          0.0
!calculated!
!toluene=C6H5#+R4CH3                  1.0E16       0.0         97.0E3
!<COLKET94>!
!calculation by KINGAS!
C6H5#+R5CHO=C6H5CHO                 5.0E12      0.0        0.0      !
estimated!
C6H5#+R10C2H3V=styrene              5.0E12      0.0        0.0      !
estimated!
C6H5#+R11C2H5=etC6H5                5.0E12      0.0        0.0      !
estimated!
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C6H5#+R3OOH=C6H5O#+R2OH              5.0E12      0.0         0.0      !
estimated!
!C6H5C3H3 n'intervient qu'ici
!C6H5#+C3H3=C6H5C3H3                  3.0E12      0.0         0.0      !
<D'ANNA98>!
C6H5#+C6H5#=biphenyl                 3.8E31     -5.75        7.9E3    !
<WANG97>!
!***disproportionnations!
C6H5#+R2OH=C6H5O#+R1H                5.0E13      0.0         0.0      !
<ALZUETA00>!
C6H5#+C6H7#=C6H6#+C6H6#              1.0E12      0.0         0.0      !
<SHANDROSS96>!

!REACTIONS OF PHENYLPEROXY RADICALS!
!***Decomposition by beta-scission!
!mfC6H5O2=OC6H4O+R1H                    2.0E13      0.0        30.0E3    !
estimated!
C6H5O2=C5H4O#+R5CHO                  2.0E13      0.0        30.0E3    !
estimated!
!see DA COSTA01!

!MF
C6H5O2+R3OOH=C6H5OOH+O2                    2.0E11          0.00  -1300
C6H5OOH=C6H5O#+R2OH                        1.5E16         0.00   43000


!REACTIONS OF PHENOXY RADICALS!
!***CO elimination!
C6H5O#=B2CO+C5H5#                     2.5E11      0.0       43.8E3    !
<BAULCH92>!
!***Combinations!
!--C6H5O#+R1H(+M)=C6H5OH#(+M)         2.5E14      0.0         0.0     !
<FRENKLACH>!
C6H5O#+R1H(+M)=C6H5OH#(+M)           1.0E14      0.0         0.0     !
estimated!
                           LOW   /1.0E94  -21.84   13.9E3/           !
<FRENKLACH>!
                           TROE /0.043 304 60000 5896/
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
C6H5O#+R1H=C5H6#+B2CO                1.1E53    -10.7         41.4E3   !
<TAN96>!
C6H5O#+B1O=OC6H4OH                    2.6E10      0.47         0.8E3   !
<LIN95>!
C6H5O#+B1O=OC6H4O+R1H                 8.5E13      0.0          0.0     !
<FRANCK94>!
C6H5O#+B1O=C5H5#+CO2                  1.0E13      0.0          0.0     !
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!
!***CO elimination!
OC6H4OH=B2CO+C5H4OH#                  7.4E11      0.0         43.8E3   !
estimated!
!as for phenoxy radicals!
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!REACTIONS OF CYCLOPENTADIENYL RADICALS!
!***Isomerization!
C5H5#=lC5H5                          1.0E14      0.0       45.5E3    !
<BRAUN89>!

!lC5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car lC5H6 n'intervient qu'ici
!lC5H5+R1H=lC5H6                     1.0E14      0.0        0.0      !
estimated!
lC5H5=C3H3+C2H2                     2.0E13      0.0        50.0E3   !
estimated!
!DH298 =43kcal/mol, Eadd=7 kcal/mol!


!***Reactions with O2!
C5H5#+O2=R5CHO+C4H4O                1.2E19     -2.48      11.0E3    !
<ZHONG98>!
!***Combinations!
C5H6# = C5H5# + R1H                          5.0E15          0.00   7.87E4
     ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>

C5H5#+B1O=C5H4O#+R1H                5.8E13     -0.02       0.02E3   !
<ZHONG98>!
C5H5#+B1O=>2C2H2+R5CHO              3.2E13     -0.17       0.44E3   !
<ZHONG98>!
C5H5#+R2OH=>C4H6Z2+B2CO              4e14       0.0         4500 !
[PENGLOAN- RODA]


C5H5#+R2OH=C5H5OH#                 1.0E13      0.0        0.0      !
calculated!
C5H5#+R3OOH=C5H5O#+R2OH              3.0E12      0.0        0.0      !
calculated!
!calculation by KINGAS!
C5H5#+C5H5#=>C10H10#                 2.0E12      0.0        0.0      !
estimated!
C10H10#=>C5H5#+C5H5#                 3.2E15      0.0        57.5E3   !
calculated!
!***disproportionnations!
C5H5#+R3OOH=>C5H6#+O2                2.5E9       1.0        3.5E3    !
estimated!
!estimated as for allylic radicals (HEYBERGER02)/10!

!REACTIONS OF CYCLOPENTADIONYL RADICALS!
!***Decompositions by beta-scission!
C5H5O#=>2C2H2+R5CHO                   2.0E13      0.0       30.0E3   !
estimated!
C5H5O#=C5H4O#+R1H                    2.0E13      0.0       30.0E3   !
estimated!
!see DA COSTA01!
!***Combinations!
C5H5O#+R1H=C5H5OH#                   1.0E14      0.0        0.0      !
estimated!
```

```
!***no disproportionnations considered!

!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!
C5H4OH#+O2=C5H4O#+R3OOH              1.0E13      0.0        5.0E3    !
estimated!
C5H4OH#+R1H=C5H5OH#                  1.0E14      0.0        0.0      !
estimated!
C5H4OH#+B1O=CO2+C2H2+R10C2H3V        3.2E13     -0.17       0.44E3   !
estimated!
!C5H4OH#+R3OOH=>R2OH+CO2+R10C2H3V+C2H2 3.0E12      0.0        0.0      !
estimated!
C5H4OH#+R3OOH=>R2OH+R2OH+C5H4O# 3.0E12      0.0        0.0      ! mf

C5H4OH#+R3OOH=>C5H5OH#+O2            2.5E9       1.0        3.5E3    !
estimated!
!Reactions derived from those of cyclopentadienyl radicals!
C5H4OH#+C6H5O#=C5H4O#+C6H5OH#        1.0E12      0.0        0.0      !
estimated!


!
*************************************************************************
*********!
!*
!*                    SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!*
!
*************************************************************************
*********!

!REACTIONS OF ORTHOBENZOQUINONE!
OC6H4O=>C5H4O#+B2CO                  1.0E12      0.0       40.0E3    !
<ALZUETA00>!
OC6H4O+R1H=>2B2CO+C2H2+R10C2H3V      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
!OC6H4O+R1H=>H2+2B2CO+C2H2+R9C2H      1.6E6       2.5        9.8E3    !
estimated!
!OC6H4O+R2OH=>H2O+2B2CO+C2H2+R9C2H    4.4E6       2.0        1.4E3    !
estimated!
!estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!
C6H5OH#=C5H6#+B2CO                   1.0E12      0.0        61.2E3   !
<HORN98>!


C6H5OH#+O2=R3OOH+C6H5O#              1.0E13     0.0       38.9E3    !
<ALZUETA00>!


C6H5OH#+B1O=OC6H4OH+R1H              1.6E13     0.0         3.4E3    !
estimated!
```

```
!as the addition of O-atoms to toluene (DACOSTA01)!
C6H5OH#+R1H=C6H5O#+H2                1.2E14     0.0       12.4E3    !
<ALZUETA00>!
C6H5OH#+B1O=C6H5O#+R2OH              1.3E13     0.0        2.9E3  !
<ALZUETA00>!
C6H5OH#+R2OH=C6H5O#+H2O              1.4E8      1.4       -0.96E3  !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H5O#+H2O2            1.0E12      0.0       10.0E3    !
<ALZUETA00>!
C6H5OH#+R4CH3=C6H5O#+CH4             1.8E11      0.0        7.7E3    !
<MULCAHY65>!
C6H5OH#+C6H5#=C6H5O#+C6H6#           4.9E12      0.0        4.4E3    !
<ALZUETA00>!
!C6H5OH#+C5H5#=C6H5O#+C5H6#          4.9E11          0.0        9.4E3    !
estimated!
!C6H5OH#+C3H5Y=C6H5O#+C3H6Y          4.9E11     0.0        9.4E3    !
estimated!
!C6H5OH#+iC4H5=C6H5O#+C4H6Z2         4.9E11          0.0        9.4E3    !
estimated!
C6H5OH#+C5H5#=C6H5O#+C5H6#           2.67e14         0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+C3H5Y=C6H5O#+C3H6Y          2.67e14     0.0        25.238e3    !mf
<Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+iC4H5=C6H5O#+C4H6Z2          2.67e14         0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>


!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!
C6H5OH#+R1H=C6H4OH#+H2               1.7E14      0.0       16.0E3    !
<SHANDROSS96>!
C6H5OH#+B1O=C6H4OH#+R2OH             2.0E13     0.0          14.7E3    !
estimated!
C6H5OH#+R2OH=C6H4OH#+H2O             1.4E13     0.0        4.6E3   !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H4OH#+H2O2           4.0E11      0.0       28.9E3    !
estimated!
C6H5OH#+R4CH3=C6H4OH#+CH4           2.0E12      0.0       15.0E3    !
estimated!
!as the H-abstractions from benzene!

C6H4OH#+O2=OC6H4OH+B1O                2.1E13      0.0       6.1E3    !
estimated!
!as for phenyl radicals (FRANCK94)!
C6H4OH#+R1H=C6H5OH#                   1.0E14      0.0       0.0      !
estimated!
C6H4OH#+R4CH3=HOC6H4CH3               5.0E12      0.0       0.0      !mf


!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!
C5H6#+O2=>C5H5#+R3OOH                1.4E12      0.0        31.6E3   !
<INGHAM94>!
!C5H6#+R1H=C5H7#                      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
```

```
C5H6#+B1O=>C5H5O#+R1H                  8.9E12     -0.15       590.0    !
<ZHONG98>!
C5H6#+R1H=C5H5#+H2                    2.8E13      0.0         2.0E3    !
<ROY97>!
C5H6#+B1O=C5H5#+R2OH                  4.8E4       2.7         1.1E3    !
<ZHONG98>!
C5H6#+R2OH=C5H5#+H2O                  3.1E6       2.0         0.0      !
<ZHONG98>!
C5H6#+R3OOH=C5H5#+H2O2                1.1E4       2.6        12.9E3    !
<ZHONG98>!
C5H6#+R4CH3=C5H5#+CH4                 1.8E-1      4.0         0.0      !
<ZHONG98>!
C5H6#+C3H5Y=C5H5#+C3H6Y              1.6E12       0.0        15.1E3    !
astoluene!
C5H6#+nC4H5=C5H5#+C4H6Z2              1.6E12      0.0        11.1E3    !
astoluene!
C5H6#+iC4H5=C5H5#+C4H6Z2              1.6E12      0.0        15.1E3    !
astoluene!
!C5H6#+C3H5Y=C5H5#+C3H6Y              6.0E12      0.0         0.0      !
estimated!
!C5H6#+nC4H5=C5H5#+C4H6Z2              6.0E12      0.0         0.0      !
estimated!
!C5H6#+iC4H5=C5H5#+C4H6Z2              6.0E12      0.0         0.0      !
<EMDEE92>!

!C5H7#=>C2H2+C3H5Y                    2.0E13      0.0        35.5E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by
HEYBERGER02!
!C5H7#+O2=C5H6#+R3OOH                  7.9E11      0.0         5.0E3    !
estimated!
!oxidation of an alkylic radical!

!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!
C5H4O#=>2C2H2+B2CO                      5.7E32     -6.76       68.5E3    !
<ALZUETA00>!
!C5H4O#=B2CO+C4H4                       1.00e12     0.0         53000    !
roda PENGLOAN!
C5H4O#+R1H=B2CO+nC4H5                  2.6E13      0.0         3.2E3    !
estimated!


!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!
C5H4O#+B1O=C4H4+CO2                    1.0E13      0.0         2.0E3     !
<ALZUETA00>!
C5H4O#+R1H=C5H3O#+H2                   8.13E7      2.031      15.88E3     !MF
idem C6H6#+R1H=C6H5#+H2
C5H4O#+B1O=C5H3O#+R2OH                 1.4E13      0.0        14.7E3     !
<ALZUETA00>!
C5H4O#+R2OH=C5H3O#+H2O                 1.1E8       1.42        1.4E3     !
<ALZUETA00>!

C5H3O#=>C2H2+B2CO+R9C2H                 2.0E13      0.0         51.0E3    !
estimated!
```

```
!estimated as the decomposition of lC6H5!
C5H3O#+O2=>CO2+C2H2+R12CHCOZ          9.7E58   -13.47       38.2E3    !
<ALZUETA00>!

C5H5OH#+R1H=C5H5O#+H2              4.0E13      0.0        6.1E3    !
<ALZUETA00>!
C5H5OH#+B1O=C5H5O#+R2OH              1.0E13      0.0        4.6E3    !
<ALZUETA00>!
C5H5OH#+R2OH=C5H5O#+H2O              1.0E13      0.0        1.7E3    !
<ALZUETA00>!

!Estimated from the same reaction for CH3OH!

C5H5OH#+R1H=C5H4OH#+H2                  1.4E13      0.0       2.0E3    !
estimated!
C5H5OH#+B1O=C5H4OH#+R2OH             4.8E4      2.7        1.1E3    !
estimated!
C5H5OH#+R2OH=C5H4OH#+H2O             1.5E6      2.0        0.0E3    !
estimated!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!
!additions decomposition
C4H4O+R1H=>R10C2H3V+CH2COZ            1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>C2H4Z+R12CHCOZ             1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>sC3H5+B2CO                 1.3E13    0.0        1.5E3     !
estimated!
C4H4O+R2OH=>C2H3CHO+R5CHO             1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+R2OH=>CO2+C3H5Y                1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+B1O=>R13CH2CHO+R12CHCOZ         6.0E4     2.56      -1.1E3     !
estimated!
C4H4O+B1O=>2CH2COZ                    6.0E4     2.56      -1.1E3     !
estimated!
!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition
C4H4O+R1H=>C2H2+R12CHCOZ+H2           8.2E5     2.5        12.3E3    !
estimated!
C4H4O+R1H=>C3H3+B2CO+H2               4.1E5     2.5         9.8E3    !
estimated!
C4H4O+R2OH=>C2H2+R12CHCOZ+H2O         2.2E6     2.0         2.8E3    !
estimated!
C4H4O+R2OH=>C3H3+B2CO+H2O             1.1E6     2.0         1.5E3    !
estimated!
C4H4O+B1O=>C2H2+R12CHCOZ+R2OH         1.2E11    0.7         8.7E3    !
estimated!
C4H4O+B1O=>C3H3+B2CO+R2OH             6.0E10    0.7         8.7E3    !
estimated!
!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!
```

```
!
!*****************************************************************************
*********!
!*                                                                 *!
!*              MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE
*!
!*                                                                 *!
!*    efficiency  coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#
and toluene*!
!*                                                                 *!
!
!*****************************************************************************
*********!

!
!*****************************************************************************
*********!
!*                                                                 *!
!*            PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE
*!
!*                                                                 *!
!
!*****************************************************************************
*********!

!*********************************!
!*REACTIONS OF TOLUENE MOLECULES*!
!*********************************!

!**UMIMOLECULAR INITITIATIONS


toluene=benzyl+R1H              2.09E15  0.0   87.51E3    !
<Oehlschlaeger07>! Zhenyu
toluene=C6H5#+R4CH3               2.66E16  0.0   97.88E3    !
<Oehlschlaeger07> Zhenyu

!**BIMOLECULAR INITITIATION
toluene+O2=benzyl+R3OOH      1.8E12   0.0    39.7E3    !<BAULCH94>!
!toluene+O2=benzyl+R3OOH      2.18e7   2.50    46045    !
mf<Oehlschlaeger06>!

!**ADDITIONS

toluene+R1H=C6H6#+R4CH3           5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet Zhenyu

toluene+B1O=OC6H4CH3+R1H      1.7E13   0.0     3.6E3    !<TAPPE89>!
!toluene+R2OH=HOC6H4CH3+R1H        2.3E12   0.0   -0.36E3   !<BAULCH92>!
toluene+R2OH=HOC6H4CH3+R1H    1.3E13   0.0    10.6E3    !<BAULCH94>as
benzene!
```

```
toluene+R2OH=C6H5OH#+R4CH3     7.83E2   2.884  3.2193E3  !Seta V Nakajima
V Miyoshi JPCA 2006 Zhenyu
!toluene+R2OH=C6H5OH#+R4CH3     1E5    2.58   1134.0    !Olive as
benzene+OH


!**METATHESES
!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

toluene+R1H=benzyl+H2         2.92E6   2.372  5.81E3   !Calcul CBS-QB3
Fournet Zhenyu
toluene+B1O=benzyl+R2OH            6.3E11   0.0       0.0   !
<HOFFMANN90>!

toluene+R2OH=benzyl+H2O            5.2E09   1.0    0.87E3   !<BAULCH94>!

toluene+R3OOH=benzyl+H2O2     4.0E11   0.0    14.0E3   !<BAULCH94>!
toluene+R4CH3=benzyl+CH4      3.91E0   3.76   6.98E3   !Calcul CBS-QB3
Fournet Zhenyu

! ajout MF
toluene+R7CH3O=benzyl+CH3OH     2.12E+10 0.0 3000.0        !PITZ2001
toluene+R8CH3OO=benzyl+CH3OOH   1.02E+04 2.5 12339.3  !PITZ2001


!toluene+R5CHO=benzyl+HCHO     3.77E13   0.0 23.7874E3    !MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO           1.26e8   1.9   18.183E3
benzyl+CH3CHO = toluene+R14CH3CO 1.26e8   1.9   18.183E3

toluene+R10C2H3V=benzyl+C2H4Z  4.0e12   0.0     8.0e3       !<COLKET94>!

toluene+C3H5Y=benzyl+C3H6Y    1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+C3H3=benzyl+pC3H4     1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2        1.6E12   0.0    15.1E3   !
<estimated(a)>!
toluene+nC4H5=benzyl+C4H6Z2        1.6E12   0.0    11.1E3   !
<estimated(a)>!
toluene+C5H5#=benzyl+C5H6#    1.6E11   0.0    15.1E3   !<estimated(a)>!
!(a) :Rate constant taken equal to that of the H-abstraction with methyl
radicals proposed !
!by COLKETT94 with A divided by 10 for cyclic radicals !
! and with an activation energy 4 kcal/mol higher for resonnance
stabilised radicals!



!ajout MF
toluene+C6H5O2=benzyl+C6H5OOH                 1.02E+04 2.5 12339.3    !
PITZ2001


toluene+C6H5#=benzyl+C6H6#    7.9E13   0.0    12.0E3   !<HECKMANN96>!
```

```
toluene+C6H5O#=benzyl+C6H5OH#         1.6E11   0.0   15.1E3 !
<estimated(a)>! peut etre trop rapide
toluene+C6H4CH3=benzyl+toluene       7.9E13   0.0   12.0E3  !
<estimated(b)>!
toluene+OC6H4CH3=benzyl+HOC6H4CH3   1.6E11   0.0   15.1E3  !
<estimated(a)>!
toluene+C6H5CH2OO=benzyl+C6H5CH2OOH 4.0E11   0.0   14.0E3  !
<estimated(c)>!
toluene+C6H5CH2O=benzyl+C6H5CH2OH    1.6E11   0.0   11.1E3 !
<estimated(a)>!
toluene+HOC6H4CH2=benzyl+HOC6H4CH3  1.6E11   0.0   15.1E3  !
<estimated(a)>!
!(b) :Rate constant taken equal to that of the H-abstraction with phenyl
radicals proposed !
!by HECKMANN96!
!(c) :Rate constant taken equal to that of the H-abstraction with HO2
radicals proposed !
!by BAULCH94!

!**METATHESES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2          1.22E08  2.031 15.88E3  !as
C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu
toluene+B1O=C6H4CH3+R2OH   2.0E13   0.0    14.7E3     !<estimated(d)>!

toluene+R2OH=C6H4CH3+H2O     1.36E4   2.7  0.6196E3   !<Seta06>! in
Sakai07 Zhenyu
toluene+R3OOH=C6H4CH3+H2O2   9.2E12   0.0   28.81E3   !<Baulch94>! in
Sakai07 Zhenyu
toluene+R4CH3=C6H4CH3+CH4   2.07E0   3.861  13.3E3    !as
C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu


!*****************************!
!*REACTIONS OF BENZYL RADICALS*!
!*****************************!

!**DECOMPOSITION BY BETA-SCISSION
benzyl=>C5H5#+C2H2             6.0E13   0.0    70.0E3 !<Colket94>!
benzyl=>C3H3+C4H4              2.0E14   0.0    83.6E3 !<Colket94>!

!**REACTIONS WITH OXYGEN
benzyl+O2=C6H5CH2OO               4.6E11   0.0   -377.0   !<FENTER94>!
benzyl+O2=C6H5CH2O+B1O         6.3E12   0.0   40.0E3  !<BREZYNSKY84>!

!**TERMINATION REACTIONS
benzyl+B1O=C6H5#+HCHO         3.5E13   0.0      0.0   !<EMDEE92>!
benzyl+B1O=C6H5CHO+R1H             1.0E14   0.0      0.0   !
<estimated(e)>!
!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4
!(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH3OO=>C6H5CH2O+R7CH3O            5.0E12     0.0        0.0
benzyl+R17C2H5OO=>C6H5CH2O+R15C2H5O        5.0E12     0.0        0.0
```

```
benzyl+R2OH=C6H5CH2OH          2.0E13   0.0      0.0  !<HIPLER91>!

!MFbenzyl+R3OOH=C6H5CH2OOH        5.0E12   0.0      0.0    !<HIPPLER92>!
benzyl+R3OOH=C6H5CH2OOH           8.21E4   2.20      -5.13E3     !MF<da
silva-bozzelli- proceedings  comb inst 32(2009)287-294>!

2benzyl=bibenzyl                    5.01E12   0.0 0.454E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3           6.1e15    0.0   75120   !<BAULCH94>!

!************************************!
!*REACTIONS OF METHYL PHENYL RADICALS*!
!************************************!

!**reactions with oxygen
!mfC6H4CH3+O2=OC6H4CH3+B1O                 2.6E13   0.0   6.1E3  !
<estimated(f)>!
!mfC6H4CH3+O2=OC6H4O+R4CH3                 3.0E13   0.0   9.0E3  !
<estimated(f)>!
!(f) : Rate constant taken equal to that of the similar reaction in the
case of phenyl!
!radicals!

!ajout mf
C6H4CH3+O2=>OOC6H4CH3                 3.72E13         -0.22      -711
     !2008DAS/BOZ3566-3575
OOC6H4CH3=>C6H4CH3+O2                 6.36E19        -1.372     48.74E3
          !2008DAS/BOZ3566-3575
OOC6H4CH3=>OC6H4CH3+B1O                     1.27E15         -0.25
     3.85E4          !2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3                     5.0E11          0.00
     46400      !



!***termination reactions!
C6H4CH3+R1H=toluene                   1.0E14   0.0   0.0    !
<estimated(g)>!
!(g) : Rate constant taken equal to that of the recombination of H atoms
with alkyl !
!radicals as proposed by Allara!


C6H4CH3+B1O=OC6H4CH3                  1.0E14   0.0   0.0    !
<estimated(f)>!
C6H4CH3+R2OH=HOC6H4CH3                1.0E13   0.0    0.0   !
<estimated(f)>!
C6H4CH3+R4CH3=C8H10#            1.2E06   1.96   -3.7E3     !
<estimation(fbis)>!
!(fbis) : Rate constant taken equal to that of the similar reaction in
the case of phenyl!
```

```
!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH           5.0E12   0.0   0.0    !
<estimated(f)>!
C6H4CH3 +R1H = benzyl + R1H           1.0E13   0.0   0.0    !<MILLER92>!

!************************************!
!*REACTIONS OF BENZYL PEROXY RADICALS*!
!************************************!


!**isomerisation-decomposition reactions
C6H5CH2OO=C6H5CHO+R2OH                      3.4E9   1.0   37.5E3  !
<estimated(h)>!
!(h) : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 23 (4 membered transition
ring)!
!+ 14.5 (secondary allylic H-atom)!

!**Combination reactions
!MF C6H5CH2OO+R1H=C6H5CH2OOH               1.0E14   0.0   0.0E3  !
<estimated(g)>!

!**dispropotionnation reactions!
C6H5CH2OO+R3OOH=C6H5CH2OOH+O2         2.0E11   0.0   -1.3E3 !
<estimated(i)>!
2C6H5CH2OO=C6H5CH2OH+C6H5CHO+O2       1.4E10   0.0   -725.0 !
<estimated(i)>!
C6H5CH2OO+C6H5CH2OO=2C6H5CH2O+O2      6.3E10   0.0   -725.0 !
<estimated(i)>!
!(i) : Rate constant taken equal to that the disproportionnation of
peroxyalkyl radicals !
!as proposed by Warth!


! ajout MF
C6H5CH2OO+R1H=C6H5CH2O+R2OH                      3.80E14         -0.19
     1.89E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=C6H5CH2OOH              4.35e60         -15.92     11.40E3
     !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=benzyl+R3OOH                  1.96E4          2.47  1.43E3
     !<da silva J Chem Theory Comput 2009>


!************************************!
!*REACTIONS OF BENZYL ALCOXY RADICALS*!
!************************************!

!**Decomposition by beta-scission ************
C6H5CH2O=R1H+C6H5CHO                        2.0E13   0.0   27.5E3 !
<estimated(j)>! INHIBE
C6H5CH2O=C6H5#+HCHO                         2.0E13   0.0   27.5E3 !
<estimated(j)>! ACCELERE
!DH = 23.59 kcal/mol!
```

```
!(j) For these beta-scissions involving the breaking of a C-C or a C-H
bond,  A-factor !
!is an average value for beta-scissions [Heyberger] and activation
energies have been!
! estimated from thermochemistry and to obtain the best results!

!C6H5CH2O=R1H+C6H5CHO                        5.26E28   -5.081   22.25E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H6#+R5CHO                        2.37E32   -6.095   28.81E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H5#+HCHO                         7.21E33   -6.21    36.85E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!

!C6H5CH2O=R1H+C6H5CHO                        1.00e14   0.00   2.91e4    !
mf<Mehl Proc comb inst 33(2011)193>!
!C6H5CH2O=C6H5#+HCHO                         1.46e20   -2.00  3.51e4    !
mf<Mehl Proc comb inst 33(2011)193>!



!***reactions with oxygen
C6H5CH2O+O2=R3OOH+C6H5CHO                    6.0E10   0.0   1.6E3  !
<estimated(k)>!
!(k) : Rate constant taken equal to that of the similar reaction in the
case of ethoxy!
!radicals as proposed by BAULCH92!

!*******************************!
!*REACTIONS OF CRESOXY RADICALS*!
!*******************************!

!**OC6H4CH3=HOC6H4CH2           2.9E9   1.0   3.2E3   !<estimated(h')>!
!(h') : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 5.9 + 5 (5 membered
transition ring)!
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2             1.1E9   1.0   22.9E3  !
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by ROO.
close bde)

!**CO elimination with rearrangement
!OC6H4CH3=>R1H+C6H6#+B2CO                  7.5E11  0.0  43.8E3 !
<FRANCK94>!
OC6H4CH3=>R1H+C6H6#+B2CO                3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>R10C2H3V+C4H4+B2CO            3.0E11  0.0  43.8E3!<FRANCK94>!
!OC6H4CH3=>C2H2+iC4H5+B2CO              3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO            3.0E11  0.0  43.8E3    !
<FRANCK94>!
OC6H4CH3=>C3H3+aC3H4+B2CO               1.5E11  0.0  43.8E3     !
<FRANCK94>!
```

```
!**termination reactions!
OC6H4CH3+R1H=HOC6H4CH3                1.0E14   0.0   0.0E3  !
<estimated(g)>!

!
**********************************************************************
*********!
!*
                                        *!
!*                    SECONDARY MECHANISM OF THE OXIDATION OF TOLUENE
            *!
!*
                                        *!
!
**********************************************************************
*********!

!************************************************!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!************************************************!

! Amorcage
!C6H5CHO+O2=C6H5CO+R3OOH         2.0E13   0.0   38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R3OOH          7.0E11   0.0   39.5E3 !RODA RODA
C6H5CHO = C6H5CO + R1H    3.98E15 0.0 83.74E3  !NIST GRELA86!

! Addition
C6H5CHO+R1H=C6H6#+R5CHO          5.8E13   0.0   8.1E3       !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13     0.0        3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the  resonnance
stabilisation of the!
! obtained radical!

C6H5CHO+B1O=C6H5CO+R2OH          6.0E12     0.0   1.8E3 !<BAULCH94>!
C6H5CHO+R2OH=C6H5CO+H2O          7.8E12     0.0   0.0   !<BAULCH94>!
C6H5CHO+R3OOH=C6H5CO+H2O2  3.0E12     0.0   11.0E3     !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4   2.0E-6     5.6   2.5E3 !MF <BAULCH94>!

C6H5CHO+R11C2H5=C6H5CO+C2H6      1.3E12     0.0   7.5E3 !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the  !
!resonnance stabilisation of the obtained radical!
```

```
C6H5CHO+C3H5Y=C6H5CO+C3H6Y 1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2     1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+nC4H5=C6H5CO+C4H6Z2     1.3E12         0.0           7.5E3      !
<estimated(p)>!
C6H5CHO+benzyl=toluene+C6H5CO         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5O#=C6H5CO+C6H5OH#         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+OC6H4CH3=C6H5CO+HOC6H4CH3     1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C5H5#=C6H5CO+C5H6#      1.3E11     0.0   11.5E3     !
<estimated(p)>
!(p) :Rate constant taken equal to that of the H-abstraction with ethyl
radicals  !
! with A divided by 10 for cyclic radicals and with an activation
energy !
!4 kcal/mol higher for resonnance stabilised radicals!

C6H5CHO+HOC6H4CH2=C6H5CO+HOC6H4CH3    1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5#=C6H5CO+C6H6#      1.3E11     0.0   11.5E3   !<estimated(p)>

C6H5CO=C6H5#+B2CO                       4E14   0.0      29.5e3   !
<SOLLY71>!
!Author(s):   Solly, R.K.; Benson, S.W.
!Title:   Kinetics of the gas-phase unimolecular decomposition of the
benzoyl radical
!Journal:   J. Am. Chem. Soc.
!Volume:   93
!Page(s):   2127
!Year:   1971

!************************************!
!*REACTIONS OF BENZYL HYDROPEROXYDE*!
!************************************!

!MFC6H5CH2OOH=C6H5CH2O+R2OH           1.5E16     0.0   42.0E3     !
<estimated(r)>!
!(r) : Rate constant taken equal to that the decomposition of
hydroperoxide species !
! proposed by Bounaceur <SAHETCHIAN>!
!MFC6H5CH2OOH=C6H5CH2O+R2OH           2.03E47         -10.27
     50.71E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OOH=C6H5CH2O+R2OH         3.29E13         0.42       39.89E3  !
MF<da silva Proc comb inst 32(2009)287-294>
C6H5CH2OOH=C6H5CHO+H2O                7.45E8          1.19
     46.04E3  !MF<da silva Proc comb inst 32(2009)287-294>


!****************************************!
!*REACTIONS OF CRESOL AND DERIVED RADICALS*!
!****************************************!
```

```
! amorcage
HOC6H4CH3+O2=OC6H4CH3+R3OOH          1.0E13     0.0   38.9E3     !
<estimated(s)>! ralenti
!A=1E13 pour phenol!
!(s) : Rate constant taken equal to that of the same reaction for
phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R3OOH        2.1E13      0.0       38.0E3    !
<EMDEE92*2>!
HOC6H4CH3+O2=HOC6H4CH2+R3OOH         2.1E12      0.0       38.6E3    !
RODA <estimated(aaa)>!

! addition
HOC6H4CH3+R1H=C6H5OH#+R4CH3             5.8E13      0.0          8.1E3
!<estimated(t)>!
!(t) : Rate constant taken equal to that of the same reaction for toluene
!

!HOC6H4CH2+B1O=C6H4OH#+HCHO 8E13 0.0 0.0




! metatheses
HOC6H4CH3+R1H=OC6H4CH3+H2          1.2E14  0.0   12.4E3     !
<estimated(s)>!
HOC6H4CH3+B1O=OC6H4CH3+R2OH             1.3E13  0.0   2.9E3 !
<estimated(s)>!
HOC6H4CH3+R2OH=OC6H4CH3+H2O           1.4E8 1.4   -0.96E3    !
<estimated(s)>!
HOC6H4CH3+R3OOH=OC6H4CH3+H2O2         1.0E12     0.0   10.0E3     !
<estimated(s)>!
HOC6H4CH3+R4CH3=OC6H4CH3+CH4          1.8E11     0.0   7.7E3 !
<estimated(s)>!
HOC6H4CH3+C6H5#=OC6H4CH3+C6H6#        4.9E12     0.0   4.4E3 !
<estimated(s)>!
HOC6H4CH3+C5H5#=OC6H4CH3+C5H6#        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2       4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH#     4.9E11     0.0   9.4E3   !
<estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2          1.2E14      0.0       8.4E3   !
<estimated(t)>!
HOC6H4CH3+B1O=HOC6H4CH2+R2OH          6.3E11         0.0
0.0     !<estimated(t)>!
HOC6H4CH3+R2OH=HOC6H4CH2+H2O          5.2E9       1.0       0.87E3  !
<estimated(t)>!
```

```
HOC6H4CH3+R3OOH=HOC6H4CH2+H2O2        4.0E11      0.0       14.0E3  !
<estimated(t)>!
HOC6H4CH3+R4CH3=HOC6H4CH2+CH4         1.6E12         0.0       11.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H5Y=HOC6H4CH2+C3H6Y 1.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H3=HOC6H4CH2+pC3H4        1.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+iC4H5=HOC6H4CH2+C4H6Z21.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+nC4H5=HOC6H4CH2+C4H6Z2      1.6E12         0.0       11.1E3  !
<estimated(t)>!
HOC6H4CH3+C5H5#=HOC6H4CH2+C5H6# 1.6E11         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C6H5#=HOC6H4CH2+C6H6# 7.9E13      0.0       12.0E3    !
<estimated(t)>!
HOC6H4CH3+C6H5O#=HOC6H4CH2+C6H5OH#    1.6E11         0.0       15.1E3   !
<estimated(t)>!
HOC6H4CH3+C6H4CH3=HOC6H4CH2+toluene   7.9E13      0.0       12.0E3   !
<estimated(t)>!
HOC6H4CH3+OC6H4CH3=HOC6H4CH2+HOC6H4CH3          1.6E11     0.0
15.1E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2OO=HOC6H4CH2+C6H5CH2OOH   4.0E11     0.0
14.0E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2O=HOC6H4CH2+C6H5CH2OH          1.6E11     0.0
11.1E3   !<estimated(t)>!

HOC6H4CH2+O2=HOC6H4CH2OO              4.6E11     0.0   -377.0     !
<estimated(u)>!
HOC6H4CH2+O2=HOC6H4CH2O+B1O           6.3E12     0.0   40.0E3     !
<estimated(u)>!
HOC6H4CH2+R3OOH=HOC6H4CH2O+R2OH       5.0E12     0.0   0.0   !
<estimated(u)>!
!(u) : Rate constant taken equal to that of the same reaction for benzyl
radicals !

HOC6H4CH2+R1H=HOC6H4CH3               1.0E14     0.0   0.0   !
<estimated(g)>!
HOC6H4CH2+R4CH3=C6H5OH#+C2H4Z         5.0E12     0.0   0.0   !
<estimated(g)>!

HOC6H4CH2OO=C6H4OHCHO+R2OH      3.4E9 1.0   37.5E3     !<estimated(v)>!
!(v) : Rate constant taken equal to that of the same reaction for benzyl
peroxy radicals !

HOC6H4CH2O=R1H+C6H4OHCHO              2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O=C6H4OH#+HCHO               2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O+O2=R3OOH+C6H4OHCHO         6.0E10      0.0       1.6E3     !
<estimated(w)>!
!(w) : Rate constant taken equal to that of the same reaction for benzyl
alcoxy radicals !
```

```
C6H4OHCHO+R1H=C6H4OHCO+H2       4.0E13     0.0   3.2E3 !<estimated(x)>!
C6H4OHCHO+B1O=C6H4OHCO+R2OH           6.0E12     0.0   1.8E3 !
<estimated(x)>!
C6H4OHCHO+R2OH=C6H4OHCO+H2O           7.8E12     0.0   0.0   !
<estimated(x)>!
C6H4OHCHO+R3OOH=C6H4OHCO+H2O2         3.0E12     0.0   11.0E3     !
<estimated(x)>!
C6H4OHCHO+R4CH3=C6H4OHCO+CH4          2.0E-6     5.6   1.5E3 !
<estimated(x)>!
!(x) : Rate constant taken equal to that of the same reaction for
benzaldehyde !

C6H4OHCO=C6H4OH#+B2CO               2.0E13 0.0   30.5E3     !
<estimated(y)>
!(y) : Rate constant taken equal to that of the same reaction for C6H5CO
radicals !

!************************************************!
!*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS*!
!************************************************!

C6H5CH2OH+O2=R3OOH+C6H5CHOH           1.4E12     0.0   34.0E3    !RODA
<estimated(aaa)>!
C6H5CH2OH+O2=C6H5CH2O+R3OOH           2.0E14     0.0   41.4E3    !
<EMDEE92>!

C6H5CH2OH+R1H=C6H6#+R6CH2OH           5.8E13  0.0     8.1E3     !
<estimated(t)>!

C6H5CH2OH+R1H=C6H5CHOH+H2       8.0E13     0.0   6.4E3 !<estimated(t')>!
C6H5CH2OH+B1O=C6H5CHOH+R2OH           4.2E11     0.0    -2.0E3   !
<estimated(t')>!
C6H5CH2OH+R2OH=C6H5CHOH+H2O           3.5E9 1.0    -1.13E3  !
<estimated(t')>!
C6H5CH2OH+R3OOH=C6H5CHOH+H2O2         2.7E11     0.0   12.0E3     !
<estimated(t')>!
C6H5CH2OH+R4CH3=C6H5CHOH+CH4          1.1E12     0.0   9.1E3 !
<estimated(t')>!
C6H5CH2OH+C3H5Y=C6H5CHOH+C3H6Y          1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+iC4H5=C6H5CHOH+C4H6Z2         1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+nC4H5=C6H5CHOH+C4H6Z2         1.112    0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C6H5#=C6H5CHOH+C6H6#        5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H4CH3=C6H5CHOH+toluene    5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H5O#=C6H5CHOH+C6H5OH#       1.1E11   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+benzyl=C6H5CHOH+toluene     1.1E11     0.0   13.1E3     !
<estimated(t')>!
C6H5CH2OH+OC6H4CH3=C6H5CHOH+HOC6H4CH3 1.1E11     0.0   13.1E3     !
<estimated(t')>!
```

```
C6H5CH2OH+HOC6H4CH2=C6H5CHOH+HOC6H4CH3     1.1E11     0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C5H5#=C6H5CHOH+C5H6#        1.1E11     0.0   13.1E3  !
<estimated(t')>!
!t': estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H                    2.0E13     0.     36.373E3    !MF
DHr=36.79 correlation baptiste E=0.6*DHr+14.3
!R15C2H5O=CH3CHO+R1H                2.0E14     0.     23.3E3 !(243,-
243)<HEICKLEN88NIST>!


!***********************************************!
!*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS*!
!***********************************************!

!** Amorзages monomolйculaires
etC6H5 = R1H + C8H9#     4.3E14 0.0 83.6E3   !<kingas>!

!** Amorзages bimolйculaires
etC6H5+O2=C8H9#+R3OOH             1.4E12   0.0   34.0E3    !
<estimated(aaa)>!
etC6H5+O2=C8H9#-1+R3OOH           1.2E13        0.0     49.0E3    !
<exgas>!

!** Additions ipso
etC6H5+R1H=C6H6#+R11C2H5           5.8E13       0.0   8.1E3    !
<estimated(t)>!

!** Metatheses
etC6H5+R1H=C8H9#+H2                   8.0E13     0.0        6.4E3
     !<estimated(t")>!
etC6H5+B1O=C8H9#+R2OH            4.2E11     0.0    -2.0                !
<estimated(t")>!
etC6H5+R2OH=C8H9#+H2O            3.5E9 1.0    -1.13E3        !
<estimated(t")>!
etC6H5+R3OOH=C8H9#+H2O2               2.7E11     0.0        12.0E3
     !<estimated(t")>!
etC6H5+R4CH3=C8H9#+CH4              1.1E12  0.0        9.1E3           !
<estimated(t")>!
etC6H5+C3H5Y=C8H9#+C3H6Y         1.1E12     0.0        13.1E3          !
<estimated(t")>!
etC6H5+iC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+nC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+C6H5O#=C8H9#+C6H5OH#     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+benzyl=C8H9#+toluene     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11     0.0        13.1E3             !
<estimated(t")>!
```

```
etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11    0.0        13.1E3          !
<estimated(t")>!
etC6H5+C5H5#=C8H9#+C5H6#        1.1E11     0.0        13.1E3          !
<estimated(t")>!

!t": estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2      7.2E8      1.5        6.79E3     !MF
correlation Dean-Bozzelli 2000
etC6H5+B1O=C8H9#-1+R2OH         5.1E8      1.5        5.05E3          !MF
correlation Dean-Bozzelli 2000
etC6H5+R2OH=C8H9#-1+H2O         3.6E6      2.0        4.82E2     !MF
correlation Dean-Bozzelli 2000
etC6H5+R3OOH=C8H9#-1+H2O2  4.2E4      2.69  1.85E4           !MF
correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4   2.43E6     1.87  1.03E4     !MF correlation
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9#        5.27E13   0.0    12.0E3  !ajout MF as
2/3 toluene <HECKMANN96>!
etC6H5+C6H5#=C6H6#+C8H9#      5.27E13   0.0    9.0E3   !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1    5.85E10   0.0    3.83E3  !ajout MF as
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>


! Ajout ipso MF
etC6H5+B1O=C6H5O#+R11C2H5  1.7E13   0.0     3.6E3    !MF as toluene !
<TAPPE89>!
etC6H5+R2OH=C6H5OH#+R11C2H5  1.3E13   0.0    10.6E3    !MF as toluene
<BAULCH94>as benzene
!etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.59E4    !MF as benzene
<Robaugh,J. Phys. Chem.90(1986)4159 - 4163>
etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.24E4    ! MF as benzene-
kcal <Robaugh,J. Phys. Chem.90(1986)4159 - 4163>

!** Decompositions

C8H9#-1=C2H4Z+C6H5#     2.0E13   0.0      35.5E3 !MF correlation exgas
C8H9#  =R1H+styrene        3.1e13   0.0      50670      !<MULLER88>
C8H9#-1=R1H+styrene        4.0E13   0.0      33.58E3    !MF <Sirjean,
J.Phys.Chem.A 2008>

!** Reactions of derived radicals
C8H9#+O2=R3OOH+styrene                      6.90E11          0.0
15.2E3      !<est (exgas-sylvain)>!

!C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO                   3.27E12          0.0
0.0      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R3OOH=R2OH+R1H+C6H5COCH3                   7.80E10          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
```

```
!C8H9#+R3OOH=>R2OH+C6H5#+CH3CHO                    2.54E11          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R3OOH=C8H9#OOH                               3.60E12          0.0
0.0    !MF KINGAS
C8H9#OOH=R2OH+C8H9#O                               5.00E15
0.0     42500          !MF
C8H9#O=R4CH3+C6H5CHO                               2.69E13          0.0
12117      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
C8H9#O=C6H5#+CH3CHO                                    1.74E14
0.0      20458         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem
81(2003)431-442>

C8H9#-1+O2=R3OOH+styrene                       2.60E11          0.0
2.5E3
C8H9#-1+R3OOH=R2OH+HCHO+benzyl                 5.00E12          0.0
0.0      !<kingas>!

!*****************************************!
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!
!*****************************************!

styrene+O2=R3OOH+C6H5C2H2          2.0E13       0.0        57.9E3  !
<asbutadiene/2>!
!C4H6Z2+O2=iC4H5+R3OOH             4.0E13       0.0        57.9E3  !
<LEUNG95>!


!styrene+B1O=C6H5#+R13CH2CHO        3.0E08       1.45        0.9E3  !
<asbutadiene/2>! ! ENLEVE PAR BENOIT ET PAG
styrene+R2OH=benzyl+HCHO           1.4E12       0.0        -0.9E3  !<as
butadiene/2!
styrene+R2OH=C6H5CHO+R4CH3         1.4E12       0.0        -0.9E3  !MF
idem rйaction prйcйdente as C3H6Y <TSAnG91>

!C4H6Z2+B1O=C3H5Y+R1H+B2CO         6.0E08       1.45        0.9E3  !
<LEUNG95,BREZINSKY84>!
!C4H6Z2+R2OH=C3H5Y+HCHO            2.8E12       0.0        -0.9E3  !
<LINSTEDT96>!
!C4H6Z2+R2OH=CH3CHO+R10C2H3V       5.6E12       0.0        -0.9E3  !
<fromLINSTEDT96>!

styrene+R1H=C6H5C2H2+H2            3.3E5        2.53        9.2E3  !MF<as
butadiene/2>!
styrene+R2OH=C6H5C2H2+H2O          1.5E6        2.0         0.4E3  !<as
butadiene/2>!
styrene+R4CH3=C6H5C2H2+CH4        3.5E13       0.0        15.5E3  !<as
butadiene/2>


!C4H6Z2+R1H=iC4H5+H2               6.6E5        2.53        9.2E3  !
<WANG97>!
!C4H6Z2+R2OH=iC4H5+H2O             3.1E6        2.0         0.4E3  !
<WANG97>!
```

```
!C4H6Z2+R4CH3=iC4H5+CH4            7.0E13       0.0        15.5E3  !
<WU87-3kcal>!

C6H5C2H2+O2=C6H5CO+HCHO            4.5E16      -1.39        1.0E3  !
<asMebel C2H3+O2>! **


!*Addition Zhenyu*!
C6H5C2H2+R1H=C6H5#C2H+H2                1.0E13       0.0
0.0  !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and
Tech. 120 (1996) 119-167.
C6H5C2H2+R2OH=C6H5#C2H+H2O         1.0E13       0.0           0.0  !in
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120
(1996) 119-167.

! ajout d'un amorcage Roda
C6H5#C2H   => C6H5# + R9C2H     2.2e16          0.0        98.0e3  ! MF
as toluene



!*****************************************!
!*REACTIONS OF C5H5CCH AND DERIVED RADICALS *!
!*****************************************!

!*Addition Zhenyu*!
!C5H5CCH=C5H5#+R9C2H                      4.2E15     0.0   125.0E3    !
<KInGAS1500>! pC3H4=R9C2H+R4CH3
!C5H5CCH+R1H=C5H5#+C2H2                  2.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R1H=C3H3+C4H4                   6.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R2OH=C5H5#+CH2COZ               4.3E11     0.0         -0.8E3
     !<BOODAGHIAnS87>!pC3H4+R2OH=CH2COZ+R4CH3
!C5H4CCH2=C5H5CCH                     2.5E12     0.0    59.0E3    !
<HIDAKA89>!aC3H4=pC3H4
!C5H4CCH2+R1H=C5H5CCH+R1H             8.5E12     0.0     2.0E3    !
<WAGnER72>!aC3H4+R1H(+M)=tC3H5(+M)
!C5H4CCH2+R2OH=C5H5#+CH2COZ           2.0E12     0.0      -0.2E3 !<LIU88>!
aC3H4+R2OH=CH2COZ+R4CH3

!*****************************************!
!*REACTIONS OF BIBENZYL AND DERIVED RADICALS*!
!*****************************************!

bibenzyl=C14H13#+R1H                  1.0E16      0.0    83.66E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
bibenzyl+O2=C14H13#+R3OOH              2.8E12      0.0     35.0E3   !<est
aaaa!
bibenzyl+R1H=C14H13#+H2                   5.4E4       2.5     -1.9E3   !
Table A-I-21 Zhenyu

bibenzyl+B1O=C14H13#+R2OH              8.4E11      0.0       -2.0   !
<estimated(t"')>!
```

```
bibenzyl+R2OH=C14H13#+H2O              7.0E9           1.0    -1.13E3   !
<estimated(t"')>!

bibenzyl+R3OOH=C14H13#+H2O2           5.4E11      0.0   12.0E3   !
<estimated(t"')>!
bibenzyl+R4CH3=C14H13#+CH4            2.2E12      0.0      9.1E3   !
<estimated(t"')>!
bibenzyl+C6H5O#=C14H13#+C6H5OH#        2.2E12      0.0     13.1e3   !
<estimated(t"')>!
bibenzyl+benzyl=C14H13#+toluene       2.2E12      0.0    9.1E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu

bibenzyl+C3H5Y=C14H13#+C3H6Y          2.2E12      0.0   13.1E3   !
<estimated(t"')>!
!t"': estimated as toluene with A x(4/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF
bibenzyl+R1H=C6H6#+C8H9#-1        5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet as toluene
bibenzyl+R2OH=C6H5OH#+C8H9#-1      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006
C14H13#=stilbene+R1H               7.94E15  0.0   51.864E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
C14H13#+O2= stilbene+R3OOH         1.6E12  0.00  15200  !as allylique
C14H13#+R3OOH=>R2OH+C6H5CHO+benzyl  8.21E4   2.20  -5.13E3 ! as benzyl

!*******************************************!
!*REACTIONS OF STILBENE                     *!
!*******************************************!
!Ajout Ipso MF
stilbene+R1H=>C6H6#+C2H2+C6H5#      5.67E8   1.43   5.65E3  !Calcul CBS-
QB3 Fournet as toluene
stilbene+R2OH=C6H5OH#+C6H5C2H2      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006

! ajout MF
stilbene+R2OH=C6H5CHO+benzyl       1.0E13       0.0        5.94E3  !
<Baulch05> as C2H4

!*************************************************!
!* Reactions of naphthalene                      *!
!*************************************************!
2C5H5#=naphthalene+H2           4.3E36  -6.3  22.835E3 ! A.M. Dean, J.
Phys. Chem. 94 (1990) 1432-1439.
C6H5#+iC4H3=naphthalene         3.18E23 -3.2  2.13E3   ! H.Y. Zhang, J.T.
McKinnon, CST 107 (1995) 261-300.
C6H5#+C4H4=naphthalene+R1H      3.3E33  -5.7  12.75E3  ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
benzyl+C3H3=>naphthalene+R1H+R1H 6.0E11  0.0  0.0      ! M.B. Colket,
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
C6H5C2H2+C2H2=naphthalene+R1H   1.6E16  -1.33 3.3E3    ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
```

```
naphthalene+O2=R3OOH+naphthyl          8.0E13      0.0        63.4E3   !
like benzene <ALZUETA00>A*8/6!
naphthalene+B1O=>indenyl+B2CO+R1H      2.7E13      0.0      3.6E3   !like
benzene <Nicovich82>A*8/6!
naphthalene+R1H=naphthyl+H2            8.0E8       1.8     16.8E3  !like
benzene <MEBEL97>A*8/6!
naphthalene+B1O=naphthyl+R2OH          2.7E13      0.0     14.7E3  !like
benzene <LINDSTEDT94>A*8/6!
naphthalene+R2OH=naphthyl+H2O          2.1E8       1.42    1.45E3  !like
benzene <BAULCH92>A*8/6!
naphthalene+R3OOH=naphthyl+H2O2        7.3E12      0.0     28.9E3  !like
benzene <BAULCH94>A*8/6!
naphthalene+R4CH3=naphthyl+CH4         2.7E12      0.0     15.0E3  !like
benzene <ZHANG89>A*8/6!

naphthyl+R1H=naphthalene          1.0E14   0.0   0.0E3  !as n-
buthylbenzene
naphthyl+O2=>indenyl+B2CO+B1O     2.6E13   0.0   6.1E3  !as n-
buthylbenzene
naphthyl+B1O=>indenyl+B2CO        1.0E14   0.0   0.0    !as n-
buthylbenzene
naphthyl+R3OOH=>indenyl+B2CO+R2OH 5.0E12   0.0   0.0    !as n-
buthylbenzene
naphthyl+R2OH=>indenyl+B2CO+R1H   1.0E13   0.0   0.0    !as n-
buthylbenzene

!************************************************!
!* Reactions of indene and derived radicals       *!
!  Indene C6H4#/CH2/CH//CH/                      *!
!  Indenyl C6H4#/CH/CH//CH/                      *!
!  ph#C3H2  C6H5#/CH(.)/C///CH                   *!
!************************************************!

indene+R2OH=>C2H4Z+C6H5CO             1.37E12  0.0  -1.04E3  !Slavinskaya
indene+R2OH=>R10C2H3V+B2CO+C6H6#      1.37E12  0.0  -1.04E3 !Est.
!indene+R2OH=>o-methylbenzyl+B2CO     1.37E12  0.0  -1.04E3

indene+O2=R3OOH+indenyl               1.4E12   0.0   31.03E3  ! as n-
buthylbenzene mais E = DH de reaction
indene+B1O=indenyl+R2OH               1.76E11  0.7   3.25E3  ! A-I-21
secondary  A*2
indene+R1H=indenyl+H2                 1.08E5   2.5   -1.9E3  ! A-I-21
secondary  A*2
indene+R2OH=indenyl+H2O               6.0E6    2.0   -1.52E3 ! A-I-21
secondary  A*2
indene+R4CH3=indenyl+CH4              2.0E11   0.0   7.3E3   ! A-I-21
secondary  A*2
indene+R3OOH=H2O2+indenyl             1.28E4   2.6   12.4E3  ! A-I-21
secondary  A*2

!indene+R1H=ph#C3H4Y         5.8E13  0.0  8.1E3  !ipso-addition
!indene+R1H=ph#C3H4-1        5.8E13  0.0  8.1E3  !ipso-addition
```

```
indene+R1H=>C2H2+benzyl       1.16E14  0.0  8.1E3 !mf 2x ipso-addition

indenyl=>C5H5#+C4H2           5.0E13   0.0  75.0E3  !Slavinskaya09
5.0E13  0.0  37.5E3
indenyl+R1H=indene           1.0E14   0.0   0.0    !as n-buthylbenzene
C6H5#+C3H3=indene            6.46E12  0.0   0.0    !Slavinskaya09
!indenyl+R3OOH=>C6H6#+B2CO+R9C2H+R2OH    3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2
indenyl+R3OOH=>C6H5#C2H+R5CHO+R2OH         3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2

indenyl+B1O=>C6H6#+B2CO+R9C2H          5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H
indenyl+B1O=>C6H5#C2H+R5CHO           5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H

indenyl+R2OH=>styrene+B2CO   4.0E14   0.0   4.5E3  !Est.
C5H5#+OH=C4H6Z2+CO

!C9H7O#=C9H6O#+R1H          2.0E13  0.0  27.5E3   ! Est.like ph#CH2O
!C9H7O#=>C6H6#+B2CO+R9C2H   2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO
!C9H7O#=C6H5#C2H+R5CHO      2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO


!END
!
!************************MPE MECHaNisM************************
!
R21CH3OCO=R4CH3+CO2                            4.840E+10    1.11
15887.0 !HuyNH aND ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                               rev / 3.570E+04    2.485   37247.0 /
R21CH3OCO=R7CH3O+B2CO                            8.020E+11    0.65
21123.0 !HuyNH aND ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                               rev / 1.350E+04    2.31     7883.0 /
!!!!!!!!!!!!!!!!!!!!
!MEtHyl EtHaNOatE    !
!!!!!!!!!!!!!!!!!!!!
!INitiatiONs
ME2j+R1H=ME                           1.000E+14   0.00       0.00   !
040909
ME=MEMj+R1H                           7.900E+15   0.00  9.797E+04   !
040909

ME=R21CH3OCO+R4CH3                       1.130E+16   0.00  7.770E+04   !
040909
!H-aBstraCtiONs
ME+R1H=ME2j+H2                        2.850E+07   2.0   7.700E+03   !
3HPalk
ME+R1H=MEMj+H2                        1.440E+13   0.00  6.095E+03   !MEOH
ME+B1O=ME2j+R2OH                        5.100E+13   0.00  7.850E+03   !
3HPalk
ME+B1O=MEMj+R2OH                        9.650E+04   2.68  3.716E+03   !2
aNC7, PriMARy f
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ME+R2OH=ME2j+H2O                        2.670E+06   2.00  4.500E+02   !
3HPalk
ME+R2OH=MEMj+H2O                        7.100E+06   1.80 -5.960E+02   !MEOH
!C-C DECOMPOsitiONs
ME2j=CH2COZ+R7CH3O                       1.280E+12   0.6584   49255.0 !
HuyNH aND ViOli J.Org.CHEM. 73 (2008) 94-101
     rev / 1.060E+02    2.7924  7922.0 /
MEMj=HCHO+R14CH3CO                       1.230E+13    0.375  36714.0 !
HuyNH aND ViOli J.Org.CHEM. 73 (2008) 94-101
                                rev / 1.110E+01    3.14   11198.0 /

!IsOMErisatiONs
ME2j=MEMj                             1.500E+08   1.00  1.980E+04   !GlauDE
Et al., ENErgy FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
!KEtONEs DECOMPOsitiON
ME2*O=CH3OH+B2CO+B2CO                   1.000E+09   0.00    40000.0   !
R5CHO+R21CH3OCO=ME2*O                    1.000E+13   0.00        0.0   !9
ALLARA aND sHaw
ME2*O+O2=ME2j*O+R3OOH                   3.000E+13   0.00    39100.0   !
ME2*O+R1H=ME2j*O+H2                     4.000E+13   0.00     4200.0   !26
aNC7; alDEHyDiC
ME2*O+R2OH=ME2j*O+H2O                   2.690E+10   0.76     -340.0   !26
aNC7: alDEHyDiC
ME2*O+B1O=ME2j*O+R2OH                     5.000E+12   0.00     1790.0   !26
aNC7; alDEHyDiC
ME2j*O=R21CH3OCO+B2CO                    1.834E+15  -0.73    22910.0   !
!!!!!!!!!!!!!!!!!!!!
!MEtHyl PrOPaNOatE   !
!!!!!!!!!!!!!!!!!!!!
!INitiatiONs
MP=MP3j+R1H            7.900E+15   0.00   9.797E+04   !as N-C4H9 DEaN Et
al., J.PHys.CHEM. 89 (1985) 4600-4608
MP2j+R1H=MP            1.000E+14   0.00   0.00        !1  rNC7*: H+fragM
MP=MPMj+R1H            7.900E+15   0.00   9.797E+04   !as N-C4H9 DEaN Et
al., J.PHys.CHEM. 89 (1985) 4600-4608

MP=ME2j+R4CH3          7.900E+22  -1.8    8.863E+04   !asC3H8 TsaNg,
J.PHys.CHEM.REf.Data 17 (1988) 887-
!H-aBstraCtiONs
MP+R1H=MP3j+H2         9.400E+04   2.75  6.280E+03   !2  aNC7, PriMARy f
MP+R1H=MP2j+H2         5.400E+04   2.5  -1.900E+03   !
MP+R1H=MPMj+H2         1.440E+13   0.00  6.095E+03   !(HELD 94)
MP+B1O=MP3j+R2OH         9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy
f
MP+B1O=MP2j+R2OH         8.800E+10   0.70  3.250E+03   !
MP+B1O=MPMj+R2OH         9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy
f
MP+R2OH=MP3j+H2O       5.250E+09   0.97  1.590E+03   !2  rNC7, PriMARy;
MP+R2OH=MP2j+H2O       3.000E+06   2.00 -1.520E+03   !
MP+R2OH=MPMj+H2O       7.100E+06   1.80 -5.960E+02   !(HELD 98)
!C-C DECOMPOsitiON
MP3j=C2H4Z+R21CH3OCO           3.030E+13   0.27   34667.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
                                rev / 1.660E+02    3.065   4838.0 /
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MP2j=CH3CHCO+R7CH3O          1.460E+12   0.61   53276.0 ! HuyNH aND ViOli
J.Org.CHEM. 73 (2008) 94-101
                                rev / 5.580E+01    2.81    5973.0 /
MPMj=HCHO+R25C2H5CO           1.230E+13   0.375  36714.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
                                rev / 1.110E+01    3.14   11198.0 /

!C-H DECOMPOsitiON
MP2D+R1H=MP3j                          4.180E+08   1.5576    1697.0 !
HuyNH aND ViOli J.Org.CHEM. 73 (2008) 94-101
     rev / 1.530E+08 1.5743 38376.0 /
MP2j=MP2D+R1H                          3.000E+13   0.00  4.550E+04   !
DayMa Et al.,INt J CHEM KiNEt, 35 (2003) 273-285 (2Hs)-5kCal
!OxiDatiONs
MP2j+R3OOH=MP2D+H2O2                   2.410E+13   0.0         0.0   !
(=NC3H7/TSA88)

!IsOMErisatiON
MP3j=MPMj                           2.500E+07   1.00  1.450E+04   !GlauDE
Et al., ENErgy FuEls, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)
    rev/   2.500E+07   1.00  1.550E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 6 + 3HP + 1kCal /O)
MP2j=MPMj                           1.500E+08   1.00  1.980E+04   !GlauDE
Et al., ENErgy FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
    rev/   1.500E+08   1.00  1.830E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 3kCal /O)
MP2D=C2H3CO2+R4CH3             3.160E+16   0.00   8.307E+04 !asDME Batt
Et al., PrOC. COMBust. INst. 19 (1982) 81-87
!H-aBstraCtiONs
MP2D+R1H=MP2DMj+H2             1.440E+13   0.0   6.095E+03   !(HELD 94)
MP2D+B1O=MP2DMj+R2OH             9.650E+04   2.68  3.716E+03   !2  aNC7,
PriMARy f
MP2D+R2OH=MP2DMj+H2O           7.100E+06   1.80 -5.960E+02   !(HELD 98)
MP2D+R1H=MP2D3j+H2             8.200E+05   2.50  1.228E+04   !TOuCHARD
MP2D+R2OH=MP2D3j+H2O           2.200E+06   2.00  2.780E+03   !TOuCHARD
MP2D+R4CH3=MP2D3j+CH4          1.360E+00   3.50  1.290E+04   !TOuCHARD
MP2D+B1O=MP2D3j+R2OH             1.200E+11   0.70  8.960E+03   !TOuCHARD
MP2D+R1H=MP2D2j+H2             4.100E+05   2.50  9.790E+03   !TOuCHARD
MP2D+R2OH=MP2D2j+H2O           1.100E+06   2.00  1.450E+03   !TOuCHARD
MP2D+R4CH3=MP2D2j+CH4          9.800E-01   3.50  1.170E+04   !TOuCHARD
MP2D+B1O=MP2D2j+R2OH             6.000E+10   0.70  7.630E+03   !TOuCHARD

!BEta-sCissiONs
MP2D3j=C2H2+R21CH3OCO           2.000E+13   0.00 4.500E+04
!MP2D3j=R21CH3OCO+C2H2           5.760E+12   0.8189 38502.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
!     rev / 1.860E+04 2.6071 6942.0 /
MP2D2j=CH2CCO+R7CH3O            5.030E+12   0.5212 48254.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
     rev / 1.850E+02 2.8060 3330.0 /
MP2DMj=C2H3CO+HCHO            2.830E+11   0.4945 29999.0 ! HuyNH aND ViOli
J.Org.CHEM. 73 (2008) 94-101
     rev / 3.190E+00 2.9288 7152.0 /
!MiB3j=C3H6Y+R21CH3OCO            2.000E+13   0.00 2.400E+04
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!IsOMErizatiONs
MP2D3j=MP2DMj              2.500E+07   1.00  1.490E+04  !GlauDE Et al.,
ENErgy FuEls, 16 (2002) 1186-1195 (CyC iNsat a 6 + 3HP)
!    rev / 1.700E+07   1.00  1.620E+04 /   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC iNsat a 6 + 2Hs + 0kCal /O)
MP2D2j=MP2DMj              1.500E+08   1.00  1.980E+04  !GlauDE Et al.,
ENErgy FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
!    rev / 9.900E+07   1.00  2.110E+04 /   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 5 + 2Hs + 0kCal /O)
MP2D2j=MP2D3j              3.120E+13   0.24  4.214E+04

!ADDitiONs
!*2
C2H3CO2=>R10C2H3V+CO2            2.200E+11   0.29  4.580E+03   !ZHOu Et
al., J.MOl.StruC.THEOCHEM. 854 (2008) 40-45
MP2D3j+O2=R5CHO+ME2*O          4.600E+16  -1.39  1.010E+03  !ST
!O aND OH DECOMPOsitiONs
MP2D+B1O=ME2j+R5CHO              1.580E+07  1.76  -1216.0   !7  MARiNOv
CalC fr
MP2D+B1O=R21CH3OCO+R13CH2CHO         5.010E+07  1.76     76.0   !7
MARiNOv CalC fr

!!!!!!!!!!!!!!!!!!!!
!MEtHyl ButaNOatE    !
!!!!!!!!!!!!!!!!!!!!
!INitiatiONs
MB=MB4j+R1H        7.900E+15   0.00   9.797E+04   !as N-C4H9 DEaN Et al.,
J.PHys.CHEM. 89 (1985) 4600-4608
MB=MB3j+R1H        5.000E+15   0.00   9.499E+04   !as s-C4H9 DEaN Et al.,
J.PHys.CHEM. 89 (1985) 4600-4608
MB2j+R1H=MB        1.000E+14   0.00   0.00        !1  rNC7*: H+fragM
MB=MBMj+R1H        7.900E+15   0.00   9.797E+04   !as N-C4H9 DEaN Et al.,
J.PHys.CHEM. 89 (1985) 4600-4608

MB=MP3j+R4CH3       7.900E+22  -1.8    8.863E+04   !asC3H8 TsaNg,
J.PHys.CHEM.REf.Data 17 (1988) 887-
MB=ME2j+R11C2H5      1.580E+17   0.0    8.704E+04   !asC4H10 TsaNg,
INt.J.CHEM.KiNEt. 10 (1978) 821-
!MB=R21CH3OCO+NC3H7   1.130E+16   0.00   8.170E+04   !asCH3COCH3 SatO Et
al., COMBust. FlaME 122 (2000) 291-311
MB=R21CH3OCO+R19C3H7   1.130E+16   0.00   8.170E+04   !asCH3COCH3 SatO Et
al., COMBust. FlaME 122 (2000) 291-311
!H-aBstraCtiONs
MB+R1H=MB4j+H2      9.400E+04   2.75  6.280E+03   !2  aNC7, PriMARy f
MB+R1H=MB3j+H2      1.300E+06   2.4   4.471E+03   !2  aNC7, sECONDARy
MB+R1H=MB2j+H2      5.400E+04   2.5  -1.900E+03   !
MB+R1H=MBMj+H2      1.440E+13   0.00   6.095E+03   !(HELD 94)
MB+B1O=MB4j+R2OH      9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy f
MB+B1O=MB3j+R2OH      4.770E+04   2.71  2.106E+03   !2  aNC7, sECONDARy
MB+B1O=MB2j+R2OH      8.800E+10   0.70  3.250E+03   !
MB+B1O=MBMj+R2OH      9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy f
MB+R2OH=MB4j+H2O      5.250E+09   0.97  1.590E+03   !2  rNC7, PriMARy;
MB+R2OH=MB3j+H2O      4.680E+07   1.61 -3.500E+01   !2  rNC7, sECONDARy
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MB+R2OH=MB2j+H2O      3.000E+06   2.00 -1.520E+03   !
MB+R4CH3=MB3j+CH4      2.705E+04   2.26  7.287E+03   !2  aNC7, sECONDARy
MB+R4CH3=MB2j+CH4      1.000E+11   0.00  7.300E+03   !
!C-C DECOMPOsitiONs
MB4j=C2H4Z+ME2j              5.250E+11    0.50   26591.0 ! HuyNH aND
ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 2.410E+02    2.89    7533.0 /
MB3j=C3H6Y+R21CH3OCO            4.530E+12    0.335  34269.0 ! HuyNH aND
ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 9.550E+01    3.05    4665.0 /
MB2j=MP2D+R4CH3               1.330E+11    0.97   34882.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
                                rev / 7.090E+02    2.78    5845.0 /
MBMj=HCHO+C3H7CO           1.230E+13    0.375  36714.0 ! HuyNH aND ViOli
J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 1.110E+01    3.14   11198.0 /
!C-H DECOMPOsitiONs
MB4j=R1H+MB3D      3.000E+13   0.00  3.800E+04   !DayMa Et al.,INt J CHEM
KiNEt, 35 (2003) 273-285 (2Hs)
MB3j=R1H+MB3D      3.000E+13   0.00  3.900E+04   !TOuCHARD Et al., INt J
CHEM KiNEt, 37 (2005) 451-463 (3HP)
MB3j=R1H+MB2D      1.500E+13   0.00  3.800E+04   !TOuCHARD (2005) THиsE
INPL (2Hs)
MB3j=R1H+MB2D-z    1.500E+13   0.00  3.800E+04   !TOuCHARD (2005) THиsE
INPL (2Hs)
!IsOMErisatiONs
MB4j=MBMj        4.350E+06   1.00  1.990E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 7 + 3HP)
!    rev/   4.350E+06   1.00  1.890E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 7 + 3HP - 1kCal /O)
MB3j=MBMj        2.500E+07   1.00  1.450E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)
    rev/   1.700E+07   1.00  1.400E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 6 + 2Hs + 2kCal /O)
MB2j=MBMj        1.500E+08   1.00  1.980E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
    rev/   1.500E+08   1.00  2.030E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 5kCal /O)
!!!!!!!!!!!!!!!!!!!!
!MEtHyl ButENOatEs   !
!!!!!!!!!!!!!!!!!!!!
!INitiatiONs
MB2D=MB3D2j+R1H                  2.500E+15    0.0    86640.0
MB2D=MP2D3j+R4CH3                1.100E+21   -1.20   97720.0 !
(TSANG91)as C3H6=C2H3+R4CH3
MB3D2j+R1H=MB3D                  1.000E+13    0.00       0.0 !(RTi)
!
!MB3D=R21CH3OCO+C3H5-a             7.940E+15    0.00  7.074E+04 !TsaNg
1978
MB3D=R21CH3OCO+C3H5Y             7.940E+15    0.00  7.074E+04 !TsaNg
1978
!H-aBstraCtiONs
MB3D+B1O=MB3D2j+R2OH          8.800E+10   0.7   3.250E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
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MB3D+B1O=MB3DMj+R2OH                              9.650E+04   2.68
3.716E+03   !2  aNC7, PriMARy f
MB3D+R1H=MB3D2j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MB3D+R1H=MB3DMj+H2                              1.440E+13   0.0   6.095E+03
!(HELD 94)
MB3D+R2OH=MB3D2j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MB3D+R2OH=MB3DMj+H2O                            7.100E+06   1.80 -5.960E+02
!(HELD 98)
MB2D+B1O=MB2DMj+R2OH                              9.650E+04   2.68
3.716E+03   !2  aNC7, PriMARy f
MB2D+R1H=MB3D2j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MB2D+R1H=MB2DMj+H2                              1.440E+13   0.0   6.095E+03
!(HELD 94)
MB2D+R2OH=MB3D2j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MB2D+R2OH=MB2DMj+H2O                            7.100E+06   1.80 -5.960E+02
!(HELD 98)
MB2D-z+B1O=MB3D2j+R2OH                            1.74E+11    0.7
5900.0
MB2D-z+B1O=MB2DMj+R2OH                            9.650E+04   2.68
3.716E+03   !2  aNC7, PriMARy f
MB2D-z+R1H=MB3D2j+H2                            1.74E+05    2.5     2510.0
MB2D-z+R1H=MB2DMj+H2                            1.440E+13   0.0   6.095E+03
!(HELD 94)
MB2D-z+R2OH=MB3D2j+H2O                          3.00E+06    2.0     -298.0
MB2D-z+R2OH=MB2DMj+H2O                          7.100E+06   1.80 -5.960E+02
!(HELD 98)
MB2D-z+R1H=MB2D3j+H2          8.200E+05   2.50  1.228E+04   !TOuCHARD
MB2D-z+R2OH=MB2D3j+H2O        2.200E+06   2.00  2.780E+03   !TOuCHARD
!IsOMErizatiONs
MB3D2j=MB3DMj          1.500E+08   1.00  2.780E+04   !GlauDE Et al.,
ENErgy FuEls, 16 (2002) 1186-1195 (X° CyC sat a 5 + 3HP)
!     rev / 9.900E+07   1.00  1.180E+04 /   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 5 + 2Htall + 0kCal /O)
MB2D3j=MB2DMj             2.500E+07   1.00  1.490E+04  !GlauDE Et al.,
ENErgy FuEls, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)
     rev / 8.600E+06   1.00  1.420E+04 /   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC iNsat a 6 + 1Ht + 0kCal /O)
MB2DMj=sC3H5CO+HCHO           2.830E+11   0.4945 29999.0 ! HuyNH aND
ViOli J.Org.CHEM. 73 (2008) 94-101
     rev / 3.190E+00 2.9288 7152.0 /
MB3DMj=HCHO+aC3H5CO         1.230E+13    0.375  36714.0 ! HuyNH aND ViOli
J. Org. CHEM. 2008 vOl. 73 PP. 94-101
     rev / 1.110E+01    3.14   11198.0 /
!
!MB2D3j=>C3H4-P+R21CH3OCO       2.000E+13   0.00   30000.0   !TOuCHARD
!
MB2D3j=>pC3H4+R21CH3OCO       2.000E+13   0.00   30000.0   !TOuCHARD
!
MB3D2j+R3OOH=>MB3D2O+R2OH             2.250E+12     0.00      0.0 !
(WALKER 90)
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MB3D2O=>ME2*O+R10C2H3V                1.700E+14    0.00   22658.0 ! Rauk
J. CaN. CHEM 2003 vOl. 81
C3H7CO=>R19C3H7+B2CO        1.834E+15  -0.73  1.291E+04   !GlauDE Et al.,
DMC C2H5CO
C3H7CO=CH2COZ+R11C2H5                2.745E+09   1.41 3.583E+04
    rev / 1.000E+04 2.48 6.130E+03 /
!!!!!!!!!!!!!!!!!!!!!
!MEtHyl PENtaNOatE   !
!!!!!!!!!!!!!!!!!!!!!
!INitiatiONs

MPE=MB4j+R4CH3       7.900E+22  -1.8    8.863E+04   !asC3H8 TsaNg,
J.PHys.CHEM.REf.Data 17 (1988) 887-
MPE=MP3j+R11C2H5      1.580E+17   0.0    8.704E+04   !asC4H10 TsaNg,
INt.J.CHEM.KiNEt. 10 (1978) 821-
MPE=ME2j+R19C3H7    1.580E+17   0.0    8.704E+04   !asC4H10 TsaNg,
INt.J.CHEM.KiNEt. 10 (1978) 821-
!
!MPE=R21CH3OCO+PC4H9   1.130E+16   0.00   8.170E+04   !asCH3COCH3 SatO Et
al., COMBust. FlaME 122 (2000) 291-311
!
NC4H9CO+R7CH3O=MPE   1.500E+13   0.00   0.00        !asDMC GlauDE Et al.,
PrOC.COMBust.INst. 31 (2005) 1111-1118
!MPE=PEaOj+R4CH3      3.160E+16   0.00   8.307E+04   !asDME Batt Et al.,
PrOC. COMBust. INst. 19 (1982) 81-87
!H-aBstraCtiONs
MPE+R1H=MPE5j+H2        9.400E+04   2.75  6.280E+03   !2  aNC7, PriMARy f
MPE+R1H=MPE4j+H2        1.300E+06   2.4   4.471E+03   !2  aNC7, sECONDARy
MPE+R1H=MPE3j+H2        1.300E+06   2.4   4.471E+03   !2  aNC7, sECONDARy
MPE+R1H=MPE2j+H2        5.400E+04   2.5  -1.900E+03   !
MPE+R1H=MPEMj+H2        1.440E+13   0.00  6.095E+03   !(HELD 94)
MPE+B1O=MPE5j+R2OH        9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy
f
MPE+B1O=MPE4j+R2OH        4.770E+04   2.71  2.106E+03   !2  aNC7,
sECONDARy
MPE+B1O=MPE3j+R2OH        4.770E+04   2.71  2.106E+03   !2  aNC7,
sECONDARy
MPE+B1O=MPE2j+R2OH        8.800E+10   0.70  3.250E+03   !
MPE+B1O=MPEMj+R2OH        9.650E+04   2.68  3.716E+03   !2  aNC7, PriMARy
f
MPE+R2OH=MPE5j+H2O      5.250E+09   0.97  1.590E+03   !2  rNC7, PriMARy;
MPE+R2OH=MPE4j+H2O      4.680E+07   1.61 -3.500E+01   !2  rNC7, sECONDARy
MPE+R2OH=MPE3j+H2O      4.680E+07   1.61 -3.500E+01   !2  rNC7, sECONDARy
MPE+R2OH=MPE2j+H2O      3.000E+06   2.00 -1.520E+03   !
MPE+R2OH=MPEMj+H2O      7.100E+06   1.80 -5.960E+02   !(HELD 98)
MPE+R4CH3=MPE4j+CH4      2.705E+04   2.26  7.287E+03   !2  aNC7,
sECONDARy
!C-C DECOMPOsitiONs
MPE5j=C2H4Z+MP3j            2.000E+13   0.00  2.870E+04   !DayMa Et
al.,INt J CHEM KiNEt, 35 (2003) 273-285
MPE4j=C3H6Y+ME2j            5.250E+11    0.50   26591.0 ! HuyNH aND ViOli
J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 2.410E+02    2.89    7533.0 /
```

```
!MPE3j=C4H8-1+R21CH3OCO        4.530E+12    0.335  34269.0 ! HuyNH aND
ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
MPE3j=C4H8Y+R21CH3OCO        4.530E+13    0.335  34269.0 ! HuyNH aND
ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 9.550E+01    3.05    4665.0 /
MPE3j=R4CH3+MB3D             2.000E+13   0.00  3.200E+04   !
MPE2j=R11C2H5+MP2D            2.000E+13   0.00  3.070E+04   !
!
!MPE2j=C4H8CO+R7CH3O           1.460E+12   0.61   53276.0 ! HuyNH aND
ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101
!                                rev / 5.580E+01    2.81    5973.0 /
MPEMj=HCHO+NC4H9CO         1.230E+13   0.375  36714.0 ! HuyNH aND ViOli
J. Org. CHEM. 2008 vOl. 73 PP. 94-101
                                rev / 1.110E+01    3.14   11198.0 /

!C-H DECOMPOsitiONs
MPE5j=R1H+MPE4D      3.000E+13   0.00  3.800E+04   !DayMa Et al.,INt J
CHEM KiNEt, 35 (2003) 273-285 (2Hs)
MPE4j=R1H+MPE4D      3.000E+13   0.00  3.900E+04   !TOuCHARD Et al., INt
J CHEM KiNEt, 37 (2005) 451-463 (3HP)
MPE4j=R1H+MPE3D      3.000E+13   0.00  3.800E+04   !DayMa Et al.,INt J
CHEM KiNEt, 35 (2003) 273-285 (2Hs)
MPE3j=R1H+MPE3D      3.000E+13   0.00  3.800E+04   !DayMa Et al.,INt J
CHEM KiNEt, 35 (2003) 273-285 (2Hs)
MPE3j=R1H+MPE2D      3.200E+13   0.00  3.480E+04   !TOuCHARD (2005) THиsE
INPL (2Hs ally)
MPE2j=R1H+MPE2D      3.000E+13   0.00  4.500E+04   !DayMa Et al.,INt J
CHEM KiNEt, 35 (2003) 273-285 (2Hs)

!IsOMErisatiONs
MPE4j=MPEMj        4.350E+06   1.00  1.990E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 7 + 3HP)
MPE3j=MPEMj        2.500E+07   1.00  1.450E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)
    rev/   1.700E+07   1.00  1.400E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 6 + 2Hs + 2kCal /O)
MPE2j=MPE5j        1.500E+08   1.00  1.980E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
MPE2j=MPEMj        1.500E+08   1.00  1.980E+04   !GlauDE Et al., ENErgy
FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)
    rev/   1.500E+08   1.00  2.030E+04/   !GlauDE Et al., ENErgy FuEls,
16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 5kCal /O)
!OxiDatiONs
MPE4j+O2=MPE3D+R3OOH    1.950E+12   0.00  5.000E+03   !BuDa Et al.,
COMBust FlaME, 142 (2005) 170-186
MPE3j+O2=MPE3D+R3OOH    1.950E+12   0.00  5.000E+03   !BuDa Et al.,
COMBust FlaME, 142 (2005) 170-186
MPE3j+O2=MPE2D+R3OOH    2.600E+11   0.00  2.500E+03   !BattiN-LEClErC,
PrOg ENErgy COMBust SCi, 34 (2008) 440-498
MPE2j+O2=MPE2D+R3OOH    1.580E+12   0.00  1.520E+04   !BattiN-LEClErC,
PrOg ENErgy COMBust SCi, 34 (2008) 440-498

!!!!!!!!!!!!!!!!!!!!!
!MEtHyl PENtENOatEs   !
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!!!!!!!!!!!!!!!!!!!!!
!INitiatiONs
!MPE4D=ME2j+C3H5-a               7.940E+15   0.00  7.074E+04 !TsaNg 1978
MPE4D=ME2j+C3H5Y               7.940E+15   0.00  7.074E+04 !TsaNg 1978
MPE3D+O2=MPE3D2j+R3OOH        4.000E+12   0.00   37000.0 !EstiMatED
MPE2D+O2=MPE3D2j+R3OOH        4.000E+12   0.00   40000.0 !as C4H8-1

!H-aBstraCtiONs
MPE4D+B1O=MPE4D2j+R2OH          8.800E+10   0.7   3.250E+03   ! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+B1O=MPE4D3j+R2OH          8.800E+10   0.7   3.250E+03   ! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+B1O=MPE3D2j+R2OH          8.800E+10   0.7   3.250E+03   ! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE2D+B1O=MPE3D2j+R2OH          8.800E+10   0.7   3.250E+03   ! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE4D+R1H=MPE4D3j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE4D+R1H=MPE4D2j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+R1H=MPE4D3j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+R1H=MPE3D2j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE2D+R1H=MPE3D2j+H2          5.400E+04   2.5  -1.900E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE4D+R2OH=MPE4D3j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE4D+R2OH=MPE4D2j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+R2OH=MPE4D3j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE3D+R2OH=MPE3D2j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
MPE2D+R2OH=MPE3D2j+H2O        3.000E+06   2.0  -1.520E+03   ! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)
!MPEXDYj raDiCals rEaCtiONs
MPE4D3j=R21CH3OCO+C4H6Z2              1.300E+13   0.00   3.590E+04   !
TOuCHARD Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (Rs+1,3-DiENE)
!
!MPE4D2j=MP2D+R10C2H3V                1.000E+12   0.00   50000.0 !
(02/09/2000)
!
MPE4D3j=MPE4D2D+R1H               3.000E+13   0.0   51500.0 !tOuCHARD
MPE4D2j=MPE4D2D+R1H               3.160E+13   0.0   34780.0 !Nist
!
NC4H9CO=>R20C4H9+B2CO               1.834e+15  -0.73  1.291e+04   !
Glaude et al., DMC C2H5CO
CH3CHCO+R2OH=R11C2H5+CO2 1.730E+12 0.00 -1.010E+03
           rev / 0.000E+00 0.00 0.000E+00 /
CH3CHCO+R1H=R11C2H5+B2CO 4.400E+12 0.00 1.459E+03
           rev / 0.000E+00 0.00 0.000E+00 /

CH3CHCO+B1O=CH3CHO+B2CO 3.200E+12 0.00 -4.370E+02
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           rev / 0.000E+00 0.00 0.000E+00 /
C2H3CO+M=>R10C2H3V+B2CO+M                      8.600E+15    0.00   23000.0
    H2O/16.25/ B2CO/1.875/ CO2/3.75/ CH4/16.25/ C2H6/16.25/

C2H3CO+R3OOH=R10C2H3V+CO2+R2OH                 2.000E+13    0.00
0.0

sC3H5CO=sC3H5+B2CO          8.600E+15 0.00 2.300E+04
           rev / 1.000E+11 0.00 6.000E+03 /

!aC3H5CO=C3H5-a+B2CO 6.199E+15 -1.09 -3.300E+02

aC3H5CO=C3H5Y+B2CO 6.199E+15 -1.09 -3.300E+02
           rev / 1.500E+11 0.00 4.810E+03 /


!!!!!!!!!!!!!!!!!!!!
!MEtHyl Hexanoate    !
!!!!!!!!!!!!!!!!!!!!

MHX=MHX6j+R1H                          7.900e+15   0.0   9.797e+04   !as
n-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=MHX5j+R1H                          5.000e+15   0.0   9.499e+04   !as
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=MHX4j+R1H                          5.000e+15   0.0   9.499e+04   !as
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=MHX3j+R1H                          5.000e+15   0.0   9.499e+04   !as
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX2j+R1H=MHX                          1.000e+14   0.0   0.0         !1
rnc7*: h +fragm
MHX=MHXmj+R1H                          7.900e+15   0.0   9.797e+04   !as
n-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608 (-4kcal prox O)
MHX=MPE5j+R4CH3                 5.000e+16   0.0   8.466e+04   !asC4H10
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=MB4j+R11C2H5                7.940e+16   0.0   8.028e+04   !asC4H10
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=MP3j+R19C3H7                7.940e+16   0.0   8.028e+04   !asC4H10
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=ME2j+R20C4H9                7.940e+16   0.0   8.028e+04   !asC4H10
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608
MHX=R21CH3OCO+R35C5H11                 1.130e+16   0.0   7.770e+04   !
asCH3COCH3 Sato et al., Combust. Flame 122 (2000) 291-311 (-4kcal prox O)
RC6H11O+R7CH3O=MHX                     1.500e+13   0.0   0.000e+00   !
asDMC Glaude et al., Proc.Combust.Inst. 31 (2005) 1111-1118
MHX=HXAoj+R4CH3                 3.160e+16   0.0   8.307e+04   !asDME Batt
et al., Proc. Combust. Inst. 19 (1982) 81-87
MHX+O2=MHX6j+R3OOH                     3.000e+13   0.0   5.280e+04   !2
anc7, primary f
MHX+O2=MHX5j+R3OOH                     2.000e+13   0.0   5.105e+04   !2
anc7, secondary
MHX+O2=MHX4j+R3OOH                     2.000e+13   0.0   5.105e+04   !2
anc7, secondary
MHX+O2=MHX3j+R3OOH                     2.000e+13   0.0   5.105e+04   !2
anc7, secondary
```

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MHX+O2=MHX2j+R3OOH                 4.000e+13   0.0   4.130e+04   !2
rnc7, tertiary
MHX+O2=MHXmj+R3OOH                 3.000e+13   0.0   5.280e+04   !2
anc7, primary f
!!!
MHX+R1H=MHX6j+H2                9.400e+04   2.75  6.280e+03   !2  anc7,
primary f
MHX+R1H=MHX5j+H2                1.300e+06   2.4   4.471e+03   !2  anc7,
secondary
MHX+R1H=MHX4j+H2                1.300e+06   2.4   4.471e+03   !2  anc7,
secondary
MHX+R1H=MHX3j+H2                1.300e+06   2.4   4.471e+03   !2  anc7,
secondary
MHX+R1H=MHX2j+H2                2.520e+14   0.0   7.300e+03   !2  rnc7,
anc7, ter
MHX+R1H=MHXmj+H2                9.400e+04   2.75  6.280e+03   !2  anc7,
primary f
MHX+B1O=MHX6j+R2OH                 9.650e+04   2.68  3.716e+03   !2
anc7, primary f
MHX+B1O=MHX5j+R2OH                 4.770e+04   2.71  2.106e+03   !2
anc7, secondary
MHX+B1O=MHX4j+R2OH                 4.770e+04   2.71  2.106e+03   !2
anc7, secondary
MHX+B1O=MHX3j+R2OH                 4.770e+04   2.71  2.106e+03   !2
anc7, secondary
MHX+B1O=MHX2j+R2OH                 2.200e+13   0.00  3.280e+03   !2
rnc7, anc7 tert
MHX+B1O=MHXmj+R2OH                 9.650e+04   2.68  3.716e+03   !2
anc7, primary f
MHX+R2OH=MHX6j+H2O                 5.250e+09   0.97  1.590e+03   !2
rnc7, primary;
MHX+R2OH=MHX5j+H2O                 4.680e+07   1.61 -3.500e+01   !2
rnc7, secondary
MHX+R2OH=MHX4j+H2O                 4.680e+07   1.61 -3.500e+01   !2
rnc7, secondary
MHX+R2OH=MHX3j+H2O                 4.680e+07   1.61 -3.500e+01   !2
rnc7, secondary
MHX+R2OH=MHX2j+H2O                 1.146e+11   0.51  6.300e+01   !2
rnc7, anc7 tert
MHX+R2OH=MHXmj+H2O                 5.250e+09   0.97  1.590e+03   !2
rnc7, primary;
MHX+R3OOH=MHX6j+H2O2            8.400e+12   0.00  2.044e+04   !2  anc7,
primary f
MHX+R3OOH=MHX5j+H2O2            5.600e+12   0.00  1.769e+04   !2  anc7,
secondary
MHX+R3OOH=MHX4j+H2O2            5.600e+12   0.00  1.769e+04   !2  anc7,
secondary
MHX+R3OOH=MHX3j+H2O2            5.600e+12   0.00  1.769e+04   !2  anc7,
secondary
MHX+R3OOH=MHX2j+H2O2            4.320e+12   0.00  1.440e+04   !2  rnc7
tertiary
MHX+R3OOH=MHXmj+H2O2            8.400e+12   0.00  2.044e+04   !2  anc7,
primary f
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```
MHX+R4CH3=MHX6j+CH4                4.520e-01   3.65  7.154e+03   !2
anc7, primary f
MHX+R4CH3=MHX5j+CH4                2.705e+04   2.26  7.287e+03   !2
anc7, secondary
MHX+R4CH3=MHX4j+CH4                2.705e+04   2.26  7.287e+03   !2
anc7, secondary
MHX+R4CH3=MHX3j+CH4                2.705e+04   2.26  7.287e+03   !2
anc7, secondary
MHX+R4CH3=MHX2j+CH4                2.000e+11   0.00  7.900e+03   !2
rnc7, anc7 tert
MHX+R4CH3=MHXmj+CH4                4.520e-01   3.65  7.154e+03   !2
anc7, primary f
MHX+R7CH3O=MHX6j+CH3OH             1.581e+11   0.00  7.000e+03   !2
rnc7, primary;
MHX+R7CH3O=MHX5j+CH3OH             1.095e+11   0.00  5.000e+03   !2
anc7, secondary
MHX+R7CH3O=MHX4j+CH3OH             1.095e+11   0.00  5.000e+03   !2
anc7, secondary
MHX+R7CH3O=MHX3j+CH3OH             1.095e+11   0.00  5.000e+03   !2
anc7, secondary
MHX+R7CH3O=MHX2j+CH3OH             3.800e+10   0.00  2.800e+03   !2
rnc7, anc7 tert
MHX+R7CH3O=MHXmj+CH3OH             1.581e+11   0.00  7.000e+03   !2
rnc7, primary;
MHX+R8CH3OO=MHX6j+CH3OOH           8.400e+12   0.00  2.044e+04   !2
corrected to ag
MHX+R8CH3OO=MHX5j+CH3OOH           5.600e+12   0.00  1.769e+04   !2
corrected to ag
MHX+R8CH3OO=MHX4j+CH3OOH           5.600e+12   0.00  1.769e+04   !2
corrected to ag
MHX+R8CH3OO=MHX3j+CH3OOH           5.600e+12   0.00  1.769e+04   !2
corrected to ag
MHX+R8CH3OO=MHX2j+CH3OOH           4.000e+12   0.00  1.400e+04   !2
same as ho2
MHX+R8CH3OO=MHXmj+CH3OOH           8.400e+12   0.00  2.044e+04   !2
corrected to ag
MHX+R10C2H3V=MHX6j+C2H4Z           5.010e+11   0.00  1.800e+04   !2
rnc7, primary;
MHX+R10C2H3V=MHX5j+C2H4Z           4.000e+11   0.00  1.680e+04   !2
rnc7, secondary
MHX+R10C2H3V=MHX4j+C2H4Z           4.000e+11   0.00  1.680e+04   !2
rnc7, secondary
MHX+R10C2H3V=MHX3j+C2H4Z           4.000e+11   0.00  1.680e+04   !2
rnc7, secondary
MHX+R10C2H3V=MHX2j+C2H4Z           4.000e+11   0.00  1.430e+04   !2
rnc7*, tertiary
MHX+R10C2H3V=MHXmj+C2H4Z           5.010e+11   0.00  1.800e+04   !2
rnc7**, primary
MHX+R11C2H5=MHX6j+C2H6             5.010e+10   0.00  1.340e+04   !2
rnc7, primary;
MHX+R11C2H5=MHX5j+C2H6             5.000e+10   0.00  1.040e+04   !2
rnc7, secondary
MHX+R11C2H5=MHX4j+C2H6             5.000e+10   0.00  1.040e+04   !2
rnc7, secondary
```

```
MHX+R11C2H5=MHX3j+C2H6                5.000e+10   0.00  1.040e+04   !2
rnc7, secondary
MHX+R11C2H5=MHX2j+C2H6                2.000e+11   0.00  7.900e+03   !2
anc7, rnc7*, te
MHX+R11C2H5=MHXmj+C2H6                5.010e+10   0.00  1.340e+04   !2
rnc7**, primary

MHX6j=MHX3j                           3.300e+09   1.00  1.730e+04   !
Glaude et al., Energy Fuels, 16 (2002) 1186-1195 Thıse INPL (cyc sat a 5
+ 2Hs)
MHX6j=MHX2j                           5.700e+08   1.00  1.000e+04   !
Glaude et al., Energy Fuels, 16 (2002) 1186-1195 Thıse INPL (cyc sat a 6
+ 2Ht)
MHX5j=MHX2j                           3.300e+09   1.00  1.530e+04   !
Glaude et al., Energy Fuels, 16 (2002) 1186-1195 Thıse INPL (cyc sat a 5
+ 2Ht)
MHX4j=MHXmj                           1.500e+08   1.00  1.990e+04   !
Glaude et al., Energy Fuels, 16 (2002) 1186-1195 Thıse INPL (cyc sat a 7
+ 3Hp)
MHX3j=MHXmj                           9.256e+10  -0.654 1.390e+04   !5
radicalc, rs fo
MHX2j=MHXmj                           8.495e+11  -0.507 2.161e+04   !5
radicalc, rs fo

MHX6j=C2H4Z+MB4j                2.000e+13   0.00  2.870e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285
MHX5j=C3H6Y+MP3j                2.000e+13   0.00  2.870e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285
MHX4j=C4H8Y+ME2j                3.300e+13   0.00  2.250e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (Y*+alcene)
MHX4j=R4CH3+MPE4D                     2.000e+13   0.00  3.100e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186
MHX3j=R11C2H5+MB3D                    2.000e+13   0.00  2.870e+04   !
Dayma et al.,Int J Chem Kinet, 35 (2003) 273-285
MHX3j=C5H10Z+R21CH3OCO                2.000e+13   0.00  3.050e+04   !
Touchard et al., Int J Chem Kinet, 37 (2005) 451-463 (-4kcal)
MHX2j=R19C3H7+MP2D                    2.000e+13   0.00  2.870e+04   !
Dayma et al.,Int J Chem Kinet, 35 (2003) 273-285
C6H10OAY+R7CH3O=MHX2j           5.000e+11   0.00 -1.000e+03   !3  anc7
:oh+c3h6=c
RC6H11O+HCHO=MHXmj              2.002e+12   0.00  2.400e+04   !3  anist:
abs val
CO2+R35C5H11=HXAoj                    1.000e+11   0.00  3.936e+04   !3
since reaction
MHX6j=R1H+MHX5d                 3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
MHX5j=R1H+MHX5d                 3.000e+13   0.00  3.900e+04   !Touchard
et al., Int J Chem Kinet, 37 (2005) 451-463 (3Hp)
MHX5j=R1H+MHX4d                 3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
MHX4j=R1H+MHX4d                 3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
MHX4j=R1H+MHX3d                 3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
```

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MHX3j=R1H+MHX3d                  3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
MHX2j=R1H+MHX2d                  3.000e+13   0.00  3.800e+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285 (2Hs)
MHX3j=R1H+MHX2d                  3.000e+13   0.00  3.750e+04   !Touchard
(2005) Thıse INPL (Ht alk)
!!!!!!
MHX5d+B1O=MHX5d4j+R2OH               8.800e+10   0.70  3.250e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX4d+B1O=MHX5d4j+R2OH               8.800e+10   0.70  3.250e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX4d+B1O=MHX4d3j+R2OH               8.800e+10   0.70  3.250e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+B1O=MHX4d3j+R2OH               8.800e+10   0.70  3.250e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+B1O=MHX3d2j+R2OH               6.800e+10   0.70  1.330e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Ht)
MHX2d+B1O=MHX3d2j+R2OH               8.800e+10   0.70  3.250e+03   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX5d+R1H=MHX5d4j+H2                 5.400e+06   2.50 -1.900e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX4d+R1H=MHX5d4j+H2                 1.740e+05   2.50  2.510e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (3Hp)
MHX4d+R1H=MHX4d3j+H2                 5.400e+06   2.50 -1.900e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+R1H=MHX4d3j+H2                 5.400e+06   2.50 -1.900e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+R1H=MHX3d2j+H2                 5.000e+04   2.50 -2.790e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Ht)
MHX2d+R1H=MHX3d2j+H2                 5.400e+06   2.50 -1.900e+03   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX5d+R2OH=MHX5d4j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX4d+R2OH=MHX5d4j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX4d+R2OH=MHX4d3j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX3d+R2OH=MHX4d3j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX3d+R2OH=MHX3d2j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX2d+R2OH=MHX3d2j+H2O               3.000e+13   0.00  1.230e+03   !6
anc7
MHX5d+R3OOH=MHX5d4j+H2O2             6.400e+03   2.60  1.240e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX4d+R3OOH=MHX5d4j+H2O2             9.600e+03   2.60  1.390e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (3Hp)
MHX4d+R3OOH=MHX4d3j+H2O2             6.400e+03   2.60  1.240e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+R3OOH=MHX4d3j+H2O2             6.400e+03   2.60  1.240e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
MHX3d+R3OOH=MHX3d2j+H2O2             3.200e+04   2.60  1.090e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Ht)
```

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MHX2d+R3OOH=MHX3d2j+H2O2              6.400e+03   2.60  1.240e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (2Hs)
!!!!!!
MHX5d+R2OH=HCHO+MPE5j           1.370e+12   0.00 -1.040e+03   !Heyberger
et al., Combust Flame, 126 (2001) 1780-1802
MHX4d+R2OH=CH3CHO+MB4j                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX3d+R2OH=C2H5CHO+MP3j               1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX2d+R2OH=C3H8CO+ME2j                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX2d+R2OH=R20C4H9+ME2*O              1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802

MHX5d4j=C4H6Z2+ME2j                   1.300e+13   0.00  3.490e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (Rs+1,3-diene)
MHX4d3j=C5H8+R21CH3OCO                1.300e+13   0.00  3.390e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (Rt+1,3-diene)
MHX3d2j=C5H8CO+R7CH3O            1.000e+13   0.00  1.500e+04   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (R+cetone/aldehyde)/2
MHX3d2j=MPE4D2D+R4CH3            6.500e+12   0.00  3.820e+04   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (CH3+1,3-diene)/2
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH2CCO
CH2CCO+R1H=C2H3CO               8.000e+11   0.00   2000.0   !
CH2CCO+R2OH=>HCCCO+H2O          2.200e+06   2.00  2.780e+03
CH2CCO+R1H=>HCCCO+H2            8.200e+05   2.50  1.228e+04
!HCCCO
HCCCO+O2=>R5CHO+B2CO+B2CO          4.600e+16  -1.39  1.010e+03  !ST
!C2H3CO
!C2H3CO+M=>R10C2H3V+B2CO+M                    8.600E+15    0.00   23000.0
END
```

The mechanism for the oxidation of fuel blend ethyl pentanoate / n-heptane/toluene.

```
ELEMENTS
H O C N AR
END
SPECIES

! Biradicals :
B1O
B2CO
B3C
B4CH
B5CH2
B6CH2

! Primary molecules :
! Reactants:
C7H16-1
C8H18-1
```

H2
H2O
O2
H2O2
CH4
HCHO
CH3OH
CO2
CH3OOH
C2H2
C2H4Z
C2H6
CH2COZ
CH3CHO
C2H5OH
C2H3OH
C2H5OOH
CH3COOOH
C3H6Y
C3H8
C4H8Y
C4H10
C2H5CHO
C3H7OH
C2H6CO
C3H8CO
C4H6Z2
C2H3CHOZ
C7H16
C8H18
C5H10Z
C7H14Z
C6H12Z
C7H14Y
C8H16Y
C8H16Z
C5H10Y
C4H10OL
C4H10O2P
C3H8O2P
C5H12
C5H10OA
C4H8OA
C5H12OL
C6H14

! Secondary molecules :
C6H12OA
C7H14OA
!C9H18Z
!C10H20Z
!C13H26Z
!C12H24Z
!C11H22Z

!C14H28Z
C8H16OA
!C9H18OA
!C12H24OA
!C11H22OA
!C10H20OA
!C13H26OA
C3H6OLY
C3H6O2PY
C4H6OAY
C4H8OLY
C6H10Y2
C7H12Y2
C10H18Y2
C11H20Y2
C8H14Y2
C4H8O2PY
C5H8OAY
C5H10OLY
!C12H22Y2
C9H16Y2
C7H14OLY
C7H14O2PY
C8H14OAY
C8H16OLY
!C14H26Y2
!C15H28Y2
C8H16O2PY
!C9H16OAY
!C9H18OLY
!C16H30Y2
!C13H24Y2
C5H10O2PY
C6H10OAY
C6H12OLY
C4H6OKZ
C5H8OKZ
C6H10OKZ
C7H12OKZ

! Cyclic primary molecules :
C2H4OE#3

! Cyclic secondary molecules :
C3H6OE#3
C4H8OE#3
C5H10OE#3
C7H14OE#3
C6H12OE#3
C8H16OE#3
!C9H18OE#3
!C10H20OE#3
!C13H26OE#3
!C12H24OE#3

```
!C11H22OE#3
!C14H28OE#3

! Benzenic primary molecules :

! Free radicals :
R1H   !   .h
R2OH   !   .oh
R3OOH   !   .o/oh
R4CH3   !   .ch3
R5CHO   !   .ch//o
R6CH2OH   !   .ch2/oh
R7CH3O   !   .o/ch3
R8CH3OO   !   .o/o/ch3
R9C2H   !   .c///ch
R10C2H3V   !   .ch//ch2
R11C2H5   !   .ch2/ch3
R12CHCOZ   !   .ch//c//o
R13CH2CHO   !   .ch2/ch//o
R14CH3CO   !   .c(//o)/ch3
R15C2H5O   !   .o/ch2/ch3
R16C2H4OOH   !   .ch2/ch2/o/oh
R17C2H5OO   !   .o/o/ch2/ch3
R18CH3COOO   !   .o/o/c(//o)/ch3
R19C3H7   !   .ch2/ch2/ch3
R20C4H9   !   .ch2/ch2/ch2/ch3
R21CH3OCO   !   .c(//o)/o/ch3
!R22CO2H   !   .c(//o)/oh
!R23C2H3O2B   !   .ch2/c(//o)/oh
!R24C2H4OH   !   .ch2/ch2/oh
!R25C2H4OH   !   .ch(/oh)/ch3
R23C2H4OH   !   c.h2-ch2-oh
R24C2H4OH   !   ch3-c.h-oh
R25C2H5CO   !   ch3-ch2-c.o

R26C7H15   !   .ch(/ch2/ch2/ch3)2
R27C7H15   !   .ch2/ch2/ch2/ch2/ch2/ch2/ch3
R28C7H15   !   .ch(/ch3)/ch2/ch2/ch2/ch2/ch3
R29C7H15   !   .ch(/ch2/ch3)/ch2/ch2/ch2/ch3
R30C8H17   !   .ch2/c(/ch3)2/ch2/ch(/ch3)2
R31C8H17   !   .ch2/ch(/ch3)/ch2/c(/ch3)3
R32C8H17   !   .c(/ch3)2/ch2/c(/ch3)3
R33C8H17   !   .ch(/ch(/ch3)2)/c(/ch3)3
R34C4H9   !   .ch(/ch3)/ch2/ch3
R35C5H11   !   .ch2/ch2/ch2/ch2/ch3
R36C4H9   !   .ch2/ch(/ch3)2
R37C5H11   !   .ch2/c(/ch3)3
R38C4H9   !   .c(/ch3)3
R39C5H11   !   .ch(/ch2/ch3)2
R40C5H11   !   .ch(/ch3)/ch2/ch2/ch3
R41C6H13   !   .ch2/ch2/ch2/ch2/ch2/ch3
R42C7H15   !   .c(/ch3)2/ch2/ch(/ch3)2
R43C3H7   !   .ch(/ch3)2
R44C7H15   !   .ch(/ch3)/ch2/c(/ch3)3
```

```
 !Cyclic free radicals:
 !Benzenic free radicals:

! lumped Free radicals :
RC3H5Y
RC4H7Y
RC3H5O
RC7H13Y
RC8H15Y
RC5H9Y
RC5H9O
RC4H7O
RC3H5O3
RC6H11O
RC7H13O
RC5H9O3
RC4H7O3
RC6H11O3
RC7H13O3
RC8H15O
!RC9H17O
!RC12H23O
!RC11H21O
!RC10H19O
!RC13H25O
RC8H15O3
!RC9H17O3
RC11H23
!RC12H23O3
RC10H21
!RC11H21O3
RC9H19
!RC10H19O3
RC12H25
!RC13H25O3
RC6H11Y
! lumped Cyclic free radicals :

N2
AR

!!!!!!!!!!Espиces rajoutйes pour le mйca toluиne

aC3H4      !ch2//ch//ch2                          propadiene = allene
pC3H4      !ch///c/ch3                                 propyne
C4H2       !ch///c/c///ch                         butadiyne = diacetylene
C4H4       !ch2//ch/c///ch                        1-buten-3-yne ou vinyl
acetylene
C4H6-12          !ch2//c//ch/ch3                       1,2-butadiиne ou
mйthyl allиne
C4H6-1           !ch///c/ch2/ch3                       1-butyne
C4H6-2           !ch3/c///c/ch3                        2-butyne
iC4H8      !ch2//c(ch3)/ch3                 2methyl-propene
C5H8       !ex ch2//ch/ch2/ch//ch2          pentadiene
```

```
iC5H8      !ex ch3/c(ch3)//c//ch2
!iC5H10          !ex ch3/ch(ch3)/ch//ch2
!C5H10           !ex ch2//ch/ch2/ch2/ch3          pentene
C5H8#      !c(#1)h2/ch2/ch//ch/ch2/1        cyclopentene
C5H6#      !c(#1)h//ch/ch//ch/ch2/1         cyclopentadiene
C6H6#      !c(#1)h&ch&ch&ch&ch&ch&1         benzene
toluene          !c(#1)h&ch&ch&ch&ch&ch&1(/ch3)
MCP              !c(#1)h2/ch2/ch//ch/ch(/ch3)/1  methylcyclopentene
MCPD       !c(#1)h//ch/ch//ch/ch(/ch3)/1   methylcyclopentadiene
C5H4O#           !o//c(#1)/ch//ch/ch//ch/1
C3H2       !.ch//c//c(.)h
C2H4O#3    !c(#1)h2/o/ch2/1
C2H3CHO          !ch(//o)/ch//ch2                 2-propenal
cC3H4      !c(#1)h2/ch//ch/1                    cyclopropene
cC3H6      !c(#1)h2/ch2/ch2/1                   cyclopropane
tC4H4      !ch2//c//c//ch2                      1,2,3 butatriene
C6H2       !ch///c/c///c/c///ch             hexatriyne
cC4H6      !c(#1)h2/ch//ch/ch2/1                cyclobutene
lC6H4      !ch///c/ch//ch/c///ch
!lC6H6           !ch2//ch/c///c/ch//ch2     !MF car n'intervient plus (une
rйaction)
lC6H8      !ch2//ch/ch//ch/ch//ch2
C6H8#      !c(#1)h2/ch//ch/ch2/ch//ch/1     cyclohexadiene
C6H10#           !c(#1)h2/ch//ch/ch2/ch2/ch2/1   cyclohexene
C8H10#           !c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1  cyclooctatriene
!Especes excitees
OHE
CHE
iC3H7      !.ch(/ch3)2
C3H3       !ch///c/ch2(.)
C3H5Y      !.ch2/ch//ch2
tC3H5      !ch2//c(.)/ch3
sC3H5      !.ch//ch/ch3
nC4H3      !.ch//ch/c///ch
iC4H3      !ch2//c(.)/c///ch
nC4H5      !.ch//ch/ch//ch2
iC4H5      !ch2//c(.)/ch//ch2
C4H5-1s          !ch///c/ch(.)/ch3
C4H5-1p          !.ch2/ch2/c///ch
C4H5-2           !.ch2/c///c/ch3
lC6H5      !ch///c/ch//ch/ch//ch(.)
lC6H7      !ex .ch//ch/ch//ch/ch//ch2
!lC6H9           !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus (une
rйaction)
C6H4#      !.c(#1)&ch&ch&ch&ch&c(.)&1
C6H5#      !.c(#1)&ch&ch&ch&ch&ch&1
C6H7#      !.c(#1)h/ch//ch/ch2/ch//ch/1
C6H9Z#           !.c(#1)h/ch//ch/ch2/ch2/ch2/1
C4H7-1           !.ch2/ch2/ch//ch2
C4H7-2           !ch3/c(.)//ch/ch3
C4H7Y      !ch3/c(.)h/ch//ch2
C4H7T      !ch2//c(.)/ch2/ch3
iC4H7      !.ch//c(/ch3)2
C4H7V      !.c(/ch3)//ch/ch3
```

```
!C5H7Y          !ch2//ch/ch//ch/c(.)h2
!iC5H7Y         !ch2//c(/c(.)h2)/ch//ch2
C5H9Y      !ch2//ch/c(.)h/ch2/ch3
iC5H9      !.ch2/ch(/ch3)/ch//ch2
!iC5H9Y         !ch3/c(.)(/ch3)/ch//ch2
CH2CHCO         !.ch2/ch//c//o
cC3H3      !.c(#1)h/ch//ch/1
! MECHANISM OF BENZENE
! Molecules
C4H4O      !ch2//ch/ch//c//o                          vinylketene
!lC5H6          !ch///c/ch//ch/ch3                          !MF car
n'intervient plus (une rйaction)
C5H5OH#         !c(#1)h//ch/ch//ch/ch(/oh)/1         cyclopentadienol
C6H5OH#         !c(#1)h&ch&ch&ch&ch&c(/oh)&1         phйnol
OC6H4O          !o//c(#1)/ch//ch/ch//ch/c(//o)/1     orthobenzoquinone
C6H5#C2H   !ch///c/c(#1)&ch&ch&ch&ch&ch/&1       phenylacetylene
etC6H5          !c(#1)h&ch&ch&ch&ch&c(/ch2/ch3)&1    ethylbenzene
styrene         !c(#1)h&ch&ch&ch&ch&c(/ch//ch2)&1
!C6H5C3H3  !c(#1)h&ch&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus
(une rйaction)
C10H10#         !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1 !
bicyclopentadienyl
C6H5CHO         !c(#1)h&ch&ch&ch&ch&c(/ch//o)&1      benzaldehyde
biphenyl   !c(#1)h&ch&ch&ch&ch&c(/c(#2)h&ch&ch&ch&ch&c&2)&1
C6H5OOH

! Radicals
C5H5#      !c(#1)(.)h/ch//ch/ch//ch/1
lC5H5      !.c///c/ch//ch/ch3
C5H3O#          !.c(#1)//ch/ch//ch/c(//o)&1
C5H5O#          !c(#1)h//ch/ch//ch/ch(/o(.))&1
C5H4OH#         !.c(#1)//ch/ch//ch/ch(/oh)&1
C6H5O#          !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5O2          !.c(#1)&ch&ch&ch&ch&c(/o/o(.))&1
C6H4OH#         !.c(#1)&ch&ch&ch&ch&c(/oh)&1
OC6H4OH         !c(#1)h&ch&ch&ch&ch(/o(.))&c(/oh)&1


!MECHANISM OF TOLUENE
HOC6H4CH3  !oh/c(#1)&ch&ch&ch&ch&c(/ch3)&1 cresol
C6H4OHCHO  !oh/c(#1)&ch&ch&ch&ch&c(/ch//o)&1
C6H5CH2OH  !c(#1)h&ch&ch&ch&ch&c(/ch2/oh)&1
C6H5CH2OOH !c(#1)h&ch&ch&ch&ch&c(/ch2/o/oh)&1
bibenzyl   !ok
stilbene   !ok
benzyl          !c(#1)h&ch&ch&ch&ch&c(/c(.)h2)&1
C6H4CH3         !c(#1)h&ch&ch&ch&ch&c(/ch3)&1
C6H4OHCO   !oh/c(#1)&ch&ch&ch&ch&c(/c(.)//o)&1
HOC6H4CH2OO !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o/o(.))&1
OC6H4CH3   !o(.)/c(#1)&ch&ch&ch&ch&c(/ch3)&1
HOC6H4CH2  !oh/c(#1)&ch&ch&ch&ch&c(/c(.)h2)&1
C6H5CO          !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5CHOH   !c(#1)h&ch&ch&ch&ch&c(/c(.)h/oh)&1
C6H5CH2O   !c(#1)h&ch&ch&ch&ch&c(/ch2/o(.))&1
```

```
HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o(.))&1
C6H5CH2OO  !c(#1)h&ch&ch&ch&ch&c(/ch2/o/o(.))&1
C8H9#      !c(#1)h&ch&ch&ch&ch&c(/c(.)h2/ch2)&1
C8H9#-1          !c(#1)h&ch&ch&ch&ch&c(/ch2/c(.)h2)&1
C6H5C2H2   !c(#1)h&ch&ch&ch&ch&c(/ch//c(.)h)&1
C14H13#          !bibenzyl -H



!MECHANISM OF CYCLOPENTENE!
!C5H8-12         !ch2//c//ch/ch2/ch3
!C5H7#           !.c(#1)h/ch2/ch//ch/ch2/1
!C5H7#Y          !c(#1)h2/c(.)h/ch//ch/ch2/1
!C5H7#V          !c(#1)h2/ch2/c(.)//ch/ch2/1
!C5H7-1s         !ch(.)//ch/ch2/ch//ch2
!C5H7-2t         !ch2//ch/ch2/c(.)//ch2
!C5H7-4t         !ch3/c(.)//ch/ch//ch2
!C5H7-3t         !ch3/ch//c(.)/ch//ch2
!C5H7-5p         !ch2(.)/ch2/ch2/c///ch
!C5H7-12-5p      !ch2(.)/ch2/ch//c//ch2
!C5H9#           !.c(#1)h/ch2/ch2/ch2/ch2/1
!C5H9      !(.)ch2/ch2/ch2/ch//ch2
!RMCP1           !c(#1)h(.)/ch2/ch//ch/ch(/ch3)/1
!RMCP2           !c(#1)h2/ch2/ch//ch/ch(/ch2(.))/1
!RMCPY1          !c(#1)h2/ch(.)/ch//ch/ch(/ch3)/1
!RMCPY2          !c(#1)h2/ch2/ch//ch/c(.)(/ch3)/1
!RMCPD           !c(#1)h//ch/ch//ch/ch(/ch2(.))/1
!RMCPDY          !c(#1)h//ch/ch//ch/c(.)(/ch3)/1

!*Especes ajoutйes*!
!mfC5H5C2H2      !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1
!C5H4CCH2  !c(#1)h//ch/ch//ch/c(//c//ch2)/1
!C5H5CCH   !c(#1)h//ch/ch//ch/ch(/c///ch)/1
!C6H5COCH3 !C6H5x/CO/CH3
C8H9#OOH   !C6H5#ch(/ooh)/ch3 ! c(#1)h&ch&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1
C8H9#O           !C6H5#ch(/o(.))/ch3 !
c(#1)h&ch&ch&ch&ch&c(/ch(/o(.))/ch3)&1
OOC6H4CH3  !o(.)/o/c(#1)&ch&ch&ch&ch&c(/ch3)&1
!C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!TolOCH2C6H5  !ch3/c(#1)&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolCH2bz      !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
CH3bzOHCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1
!Benzaldtol       !
c(#1)h&ch&ch&ch&ch&c(/c(//o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1
!HOC6H4CHO  !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1
!C6H5C4H7   !c(#1)h&ch&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1
naphthalene
!benzofuran
C8H8O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2
C8H7O#          ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch(.)/ch2/2
C8H7O#-1        ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch(.)/2
naphthyl
indenyl
```

```
indene
!cumene
!CH3styre
C9H11#-1
C2H3C6H4CH2
!phenanthrene
!C6H5CH2CHO
!!!!!!!!!!!!!!!!!!!!!!!!!
**************************************************************************
!!!!!Ethyl esters
EF
HCOOH
C2H5OCO
EFEJ
EFMJ
EFED
CH2OCHO
CH3COOH
EA2J
EA
EA2J
EAEJ
EAMJ
MEMJ
EAEJ
EAMJ
EAED
HOCO
CH2COOH
EP
C2H5COOH
EP3J
EP2J
EPEJ
EPMJ
C2H5CO
MPMJ
CH3CHCO
EP2d
EPED
CH2CH2COOH
CH3CHCOOH
C2H3COOH
EB
C3H7COOH
EB4J
EB3J
EB2J
EBEJ
EBMJ
NC3H7CO
MBMJ
C2H5CHCO
EB3D
```

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EB2D
EBed
PRCOOH-4
PRCOOH-3
PRCOOH-2
C3H5COOH
EPE
C4H9COOH
EPE5J
EPE4J
EPE3J
EPE2J
EPEEJ
EPEMJ
EPE4D
EPE3D
EPE2D
EPEED
NC4H9CO
MPEMJ
C4H8CO
BUCOOH-5
BUCOOH-4
BUCOOH-3
BUCOOH-2
C4H7COOH
HCO2
CH3CO2
C2H5CO2
C3H7CO2
C4H9CO2
C3H7COCO2
CH3COCO2
CH3CHCHO
NC3H7CHO
END


REACTIONS
(k = A T**b exp(-E/RT)) A units: mole-cm-sec-K, E units cal/mole)

!     -----------------
!     PRIMARY REACTIONS
!     -----------------
!   molecular elimination :
!   unimolecular initiations :
C7H16-1=>R19C3H7+R20C4H9    2.0E+0017  0.000  85750.3  ! UI 1 KB
C7H16-1=>R11C2H5+R35C5H11    1.6E+0017  0.000  85815.5  ! UI 2 KB
C7H16-1=>R4CH3+R41C6H13    3.2E+0017  0.000  87654.8  ! UI 3 KB
C8H18-1=>R4CH3+R42C7H15    1.2E+0018  0.000  81845.9  ! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9    2.4E+0017  0.000  78804.1  ! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11    4.6E+0017  0.000  83562.0  ! UI 6 KB
C8H18-1=>R4CH3+R44C7H15    8.0E+0017  0.000  87665.1  ! UI 7 KB
```

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!   bimolecular initiations :
C7H16-1+O2=>R3OOH+R26C7H15    1.4E+0013  0.000  50652.5  ! BI 8 CN
C7H16-1+O2=>R3OOH+R27C7H15    4.2E+0013  0.000  53033.1  ! BI 9 CN
C7H16-1+O2=>R3OOH+R28C7H15    2.8E+0013  0.000  50588.2  ! BI 10 CN
C7H16-1+O2=>R3OOH+R29C7H15    2.8E+0013  0.000  50652.5  ! BI 11 CN
C8H18-1+O2=>R3OOH+R30C8H17    6.3E+0013  0.000  53033.0  ! BI 12 CN
C8H18-1+O2=>R3OOH+R31C8H17    4.2E+0013  0.000  52333.1  ! BI 13 CN
C8H18-1+O2=>R3OOH+R32C8H17    7.0E+0012  0.000  47243.3  ! BI 14 CN
C8H18-1+O2=>R3OOH+R33C8H17    1.4E+0013  0.000  50652.7  ! BI 15 CN

!   additions :

!   additions with oxygen:

!   isomerisations :
R20C4H9=R34C4H9    3.3E+0009  1.000  37000.0  ! IS 16 KB
R26C7H15=R28C7H15    6.7E+0009  1.000  37000.0  ! IS 17 KB
R26C7H15=R27C7H15    1.7E+0009  1.000  19800.0  ! IS 18 KB
R27C7H15=R29C7H15    9.9E+0007  1.000  37000.0  ! IS 19 KB
R27C7H15=R28C7H15    1.7E+0007  1.000  17400.0  ! IS 20 KB
R28C7H15=R29C7H15    5.7E+0008  1.000  17300.0  ! IS 21 KB
R30C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 22 KB
R30C8H17=R32C8H17    2.9E+0008  1.000  15300.0  ! IS 23 KB
R30C8H17=R31C8H17    3.0E+0008  1.000  14500.0  ! IS 24 KB
R31C8H17=R33C8H17    3.3E+0009  1.000  37000.0  ! IS 25 KB
R35C5H11=R39C5H11    3.3E+0009  1.000  37000.0  ! IS 26 KB
R35C5H11=R40C5H11    5.7E+0008  1.000  17300.0  ! IS 27 KB

!   Decomposition of OOQOOH into branching agents:

!   beta-scissions :
R19C3H7=>R4CH3+C2H4Z    2.0E+0013  0.000  31000.0  ! DE 28 CN
R19C3H7=>R1H+C3H6Y    3.0E+0013  0.000  38000.0  ! DE 29 CN
R20C4H9=>R11C2H5+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 30 CW
R20C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 31 CN
R26C7H15=>R11C2H5+C5H10Z    4.0E+0013  0.000  28700.0  ! DE 32 CW
R26C7H15=>R1H+C7H14Z    6.0E+0013  0.000  38000.0  ! DE 33 CN
R27C7H15=>R35C5H11+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 34 CW
R27C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 35 CN
R28C7H15=>R20C4H9+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 36 CW
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 37 CN
     DUPLICATE
R28C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 38 CN
     DUPLICATE
R29C7H15=>R19C3H7+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 39 CW
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 40 CN
     DUPLICATE
R29C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 41 CN
     DUPLICATE
R29C7H15=>R4CH3+C6H12Z    2.0E+0013  0.000  31000.0  ! DE 42 CN
R30C8H17=>R36C4H9+C4H8Y    2.0E+0013  0.000  28700.0  ! DE 43 CW
R30C8H17=>R4CH3+C7H14Y    4.0E+0013  0.000  31000.0  ! DE 44 CN
R31C8H17=>R37C5H11+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 45 CW
R31C8H17=>R4CH3+C7H14Z    2.0E+0013  0.000  31000.0  ! DE 46 CN
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R31C8H17=>R1H+C8H16Y    1.5E+0013  0.000  37500.0  ! DE 47 CN
R32C8H17=>R38C4H9+C4H8Y    2.0E+0013  0.000  26700.0  ! DE 48
R32C8H17=>R1H+C8H16Y    6.0E+0013  0.000  39000.0  ! DE 49 CN
R32C8H17=>R1H+C8H16Z    3.0E+0013  0.000  38000.0  ! DE 50 CN
R33C8H17=>R4CH3+C7H14Z    4.0E+0013  0.000  31000.0  ! DE 51 CN
R33C8H17=>R4CH3+C7H14Y    6.0E+0013  0.000  31000.0  ! DE 52 CN
R33C8H17=>R1H+C8H16Z    3.0E+0013  0.000  37500.0  ! DE 53 CN
R34C4H9=>R4CH3+C3H6Y    2.0E+0013  0.000  31000.0  ! DE 54 CN
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  38000.0  ! DE 55 CN
     DUPLICATE
R34C4H9=>R1H+C4H8Y    3.0E+0013  0.000  39000.0  ! DE 56 CN
     DUPLICATE
R35C5H11=>R19C3H7+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 57 CW
R35C5H11=>R1H+C5H10Z    3.0E+0013  0.000  38000.0  ! DE 58 CN
R36C4H9=>R4CH3+C3H6Y    4.0E+0013  0.000  31000.0  ! DE 59 CN
R36C4H9=>R1H+C4H8Y    3.0E+0013  0.000  37500.0  ! DE 60 CN
R37C5H11=>R4CH3+C4H8Y    6.0E+0013  0.000  31000.0  ! DE 61 CN
R38C4H9=>R1H+C4H8Y    9.0E+0013  0.000  39000.0  ! DE 62 CN
R39C5H11=>R4CH3+C4H8Y    4.0E+0013  0.000  31000.0  ! DE 63 CN
R39C5H11=>R1H+C5H10Y    6.0E+0013  0.000  38000.0  ! DE 64 CN
R40C5H11=>R11C2H5+C3H6Y    2.0E+0013  0.000  28700.0  ! DE 65 CW
R40C5H11=>R1H+C5H10Z    3.0E+0013  0.000  39000.0  ! DE 66 CN
R40C5H11=>R1H+C5H10Y    3.0E+0013  0.000  38000.0  ! DE 67 CN
R41C6H13=>R20C4H9+C2H4Z    2.0E+0013  0.000  28700.0  ! DE 68 CW
R41C6H13=>R1H+C6H12Z    3.0E+0013  0.000  38000.0  ! DE 69 CN
R42C7H15=>R43C3H7+C4H8Y    2.0E+0013  0.000  27700.0  ! DE 70
R42C7H15=>R1H+C7H14Y    3.0E+0013  0.000  38000.0  ! DE 71 CN
     DUPLICATE
R42C7H15=>R1H+C7H14Y    6.0E+0013  0.000  39000.0  ! DE 72 CN
     DUPLICATE
R43C3H7=>R1H+C3H6Y    6.0E+0013  0.000  39000.0  ! DE 73 CN
R44C7H15=>R38C4H9+C3H6Y    2.0E+0013  0.000  26700.0  ! DE 74
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  38000.0  ! DE 75 CN
     DUPLICATE
R44C7H15=>R1H+C7H14Z    3.0E+0013  0.000  39000.0  ! DE 76 CN
     DUPLICATE
! decomposition of R(.)CO free radicals

!   decomposition to o-rings :

!   oxidations :
R26C7H15+O2=>C7H14Z+R3OOH    3.9E+0012  0.000  5000.0  ! OX 77 CN
R27C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 78 CN
R28C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 79 CN
     DUPLICATE
R28C7H15+O2=>C7H14Z+R3OOH    8.1E+0011  0.000  5000.0  ! OX 80 CN
     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 81 CN
     DUPLICATE
R29C7H15+O2=>C7H14Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 82 CN
     DUPLICATE
R31C8H17+O2=>C8H16Y+R3OOH    6.4E+0011  0.000  5000.0  ! OX 83 CN
R32C8H17+O2=>C8H16Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 84 CN
R32C8H17+O2=>C8H16Z+R3OOH    1.9E+0012  0.000  5000.0  ! OX 85 CN
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R33C8H17+O2=>C8H16Z+R3OOH    6.4E+0011  0.000  5000.0  ! OX 86 CN
R38C4H9+O2=>C4H8Y+R3OOH    1.6E+0012  0.000  5000.0  ! OX 87 CW
R43C3H7+O2=>C3H6Y+R3OOH    2.3E+0012  0.000  5000.0  ! OX 88 CW

!   oxidations of R(.)(OH) radicals:

!   metathesis :
B1O+C7H16-1=>R2OH+R26C7H15    2.6E+0013  0.000  5200.0  ! ME 89 CW
B1O+C7H16-1=>R2OH+R27C7H15    1.0E+0014  0.000  7850.0  ! ME 90 CW
B1O+C7H16-1=>R2OH+R28C7H15    5.2E+0013  0.000  5200.0  ! ME 91 CW
B1O+C7H16-1=>R2OH+R29C7H15    5.2E+0013  0.000  5200.0  ! ME 92 CW
B1O+C8H18-1=>R2OH+R30C8H17    1.5E+0014  0.000  7850.0  ! ME 93 CW
B1O+C8H18-1=>R2OH+R31C8H17    1.0E+0014  0.000  7850.0  ! ME 94 CW
B1O+C8H18-1=>R2OH+R32C8H17    1.0E+0013  0.000  3280.0  ! ME 95 CW
B1O+C8H18-1=>R2OH+R33C8H17    2.6E+0013  0.000  5200.0  ! ME 96 CW
C7H16-1+R1H=>H2+R26C7H15    9.0E+0006  2.000  5000.0  ! ME 97 CW
C7H16-1+R1H=>H2+R27C7H15    5.7E+0007  2.000  7700.0  ! ME 98 CW
C7H16-1+R1H=>H2+R28C7H15    1.8E+0007  2.000  5000.0  ! ME 99 CW
C7H16-1+R1H=>H2+R29C7H15    1.8E+0007  2.000  5000.0  ! ME 100 CW
C8H18-1+R1H=>H2+R30C8H17    8.6E+0007  2.000  7700.0  ! ME 101 CW
C8H18-1+R1H=>H2+R31C8H17    5.7E+0007  2.000  7700.0  ! ME 102 CW
C8H18-1+R1H=>H2+R32C8H17    4.2E+0006  2.000  2400.0  ! ME 103 CN
C8H18-1+R1H=>H2+R33C8H17    9.0E+0006  2.000  5000.0  ! ME 104 CW
C7H16-1+R2OH=>H2O+R26C7H15    2.6E+0006  2.000  -765.0  ! ME 105 CW
C7H16-1+R2OH=>H2O+R27C7H15    5.4E+0006  2.000  450.0  ! ME 106 CW
C7H16-1+R2OH=>H2O+R28C7H15    5.2E+0006  2.000  -765.0  ! ME 107 CW
C7H16-1+R2OH=>H2O+R29C7H15    5.2E+0006  2.000  -765.0  ! ME 108 CW
C8H18-1+R2OH=>H2O+R30C8H17    8.1E+0006  2.000  450.0  ! ME 109 CW
C8H18-1+R2OH=>H2O+R31C8H17    5.4E+0006  2.000  450.0  ! ME 110 CW
C8H18-1+R2OH=>H2O+R32C8H17    1.1E+0006  2.000  -1865.0  ! ME 111 CW
C8H18-1+R2OH=>H2O+R33C8H17    2.6E+0006  2.000  -765.0  ! ME 112 CW
C7H16-1+R3OOH=>H2O2+R26C7H15    4.0E+0011  0.000  15500.0  ! ME 113 CN
C7H16-1+R3OOH=>H2O2+R27C7H15    1.2E+0012  0.000  17000.0  ! ME 114 CN
C7H16-1+R3OOH=>H2O2+R28C7H15    8.0E+0011  0.000  15500.0  ! ME 115 CN
C7H16-1+R3OOH=>H2O2+R29C7H15    8.0E+0011  0.000  15500.0  ! ME 116 CN
C8H18-1+R3OOH=>H2O2+R30C8H17    1.8E+0012  0.000  17000.0  ! ME 117 CN
C8H18-1+R3OOH=>H2O2+R31C8H17    1.2E+0012  0.000  17000.0  ! ME 118 CN
C8H18-1+R3OOH=>H2O2+R32C8H17    2.0E+0011  0.000  14000.0  ! ME 119 CN
C8H18-1+R3OOH=>H2O2+R33C8H17    4.0E+0011  0.000  15500.0  ! ME 120 CN
C7H16-1+R4CH3=>CH4+R26C7H15    2.0E+0011  0.000  9600.0  ! ME 121 CN
C7H16-1+R4CH3=>CH4+R27C7H15    6.0E-0001  4.000  8200.0  ! ME 122 CN
C7H16-1+R4CH3=>CH4+R28C7H15    4.0E+0011  0.000  9600.0  ! ME 123 CN
C7H16-1+R4CH3=>CH4+R29C7H15    4.0E+0011  0.000  9600.0  ! ME 124 CN
C8H18-1+R4CH3=>CH4+R30C8H17    9.0E-0001  4.000  8200.0  ! ME 125 CN
C8H18-1+R4CH3=>CH4+R31C8H17    6.0E-0001  4.000  8200.0  ! ME 126 CN
C8H18-1+R4CH3=>CH4+R32C8H17    1.0E+0011  0.000  7900.0  ! ME 127 CW
C8H18-1+R4CH3=>CH4+R33C8H17    2.0E+0011  0.000  9600.0  ! ME 128 CN
C7H16-1+R5CHO=>HCHO+R26C7H15    1.0E+0007  1.900  17000.0  ! ME 129 CN
C7H16-1+R5CHO=>HCHO+R27C7H15    2.0E+0005  2.500  18500.0  ! ME 130 CN
C7H16-1+R5CHO=>HCHO+R28C7H15    2.2E+0007  1.900  17000.0  ! ME 131 CN
C7H16-1+R5CHO=>HCHO+R29C7H15    2.2E+0007  1.900  17000.0  ! ME 132 CN
C8H18-1+R5CHO=>HCHO+R30C8H17    3.1E+0005  2.500  18500.0  ! ME 133 CN
C8H18-1+R5CHO=>HCHO+R31C8H17    2.0E+0005  2.500  18500.0  ! ME 134 CN
C8H18-1+R5CHO=>HCHO+R32C8H17    3.4E+0004  2.500  13500.0  ! ME 135 CN
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C8H18-1+R5CHO=>HCHO+R33C8H17    1.0E+0007  1.900  17000.0  ! ME 136 CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15    6.0E+0001  2.950  12000.0  ! ME 137 CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15    2.0E+0002  2.950  14000.0  ! ME 138 CN
C7H16-1+R6CH2OH=>CH3OH+R28C7H15    1.2E+0002  2.950  12000.0  ! ME 139 CN
C7H16-1+R6CH2OH=>CH3OH+R29C7H15    1.2E+0002  2.950  12000.0  ! ME 140 CN
C8H18-1+R6CH2OH=>CH3OH+R30C8H17    3.0E+0002  2.950  14000.0  ! ME 141 CN
C8H18-1+R6CH2OH=>CH3OH+R31C8H17    2.0E+0002  2.950  14000.0  ! ME 142 CN
C8H18-1+R6CH2OH=>CH3OH+R32C8H17    1.2E+0002  2.760  10800.0  ! ME 143 CN
C8H18-1+R6CH2OH=>CH3OH+R33C8H17    6.0E+0001  2.950  12000.0  ! ME 144 CN
C7H16-1+R7CH3O=>CH3OH+R26C7H15    1.5E+0011  0.000  4500.0  ! ME 145 CN
C7H16-1+R7CH3O=>CH3OH+R27C7H15    3.2E+0011  0.000  7300.0  ! ME 146 CN
C7H16-1+R7CH3O=>CH3OH+R28C7H15    2.9E+0011  0.000  4500.0  ! ME 147 CN
C7H16-1+R7CH3O=>CH3OH+R29C7H15    2.9E+0011  0.000  4500.0  ! ME 148 CN
C8H18-1+R7CH3O=>CH3OH+R30C8H17    4.9E+0011  0.000  7300.0  ! ME 149 CN
C8H18-1+R7CH3O=>CH3OH+R31C8H17    3.2E+0011  0.000  7300.0  ! ME 150 CN
C8H18-1+R7CH3O=>CH3OH+R32C8H17    2.3E+0010  0.000  2900.0  ! ME 151 CN
C8H18-1+R7CH3O=>CH3OH+R33C8H17    1.5E+0011  0.000  4500.0  ! ME 152 CN
C7H16-1+R8CH3OO=>CH3OOH+R26C7H15    3.0E+0012  0.000  17500.0  ! ME 153
CN
C7H16-1+R8CH3OO=>CH3OOH+R27C7H15    1.2E+0013  0.000  20000.0  ! ME 154
CN
C7H16-1+R8CH3OO=>CH3OOH+R28C7H15    6.0E+0012  0.000  17500.0  ! ME 155
CN
C7H16-1+R8CH3OO=>CH3OOH+R29C7H15    6.0E+0012  0.000  17500.0  ! ME 156
CN
C8H18-1+R8CH3OO=>CH3OOH+R30C8H17    1.8E+0013  0.000  20000.0  ! ME 157
CN
C8H18-1+R8CH3OO=>CH3OOH+R31C8H17    1.2E+0013  0.000  20000.0  ! ME 158
CN
C8H18-1+R8CH3OO=>CH3OOH+R32C8H17    1.5E+0012  0.000  15000.0  ! ME 159
CN
C8H18-1+R8CH3OO=>CH3OOH+R33C8H17    3.0E+0012  0.000  17500.0  ! ME 160
CN
C7H16-1+R11C2H5=>C2H6+R26C7H15    2.0E+0011  0.000  11000.0  ! ME 161 CN
C7H16-1+R11C2H5=>C2H6+R27C7H15    6.0E+0011  0.000  13500.0  ! ME 162 CR
C7H16-1+R11C2H5=>C2H6+R28C7H15    4.0E+0011  0.000  11000.0  ! ME 163 CN
C7H16-1+R11C2H5=>C2H6+R29C7H15    4.0E+0011  0.000  11000.0  ! ME 164 CN
C8H18-1+R11C2H5=>C2H6+R30C8H17    9.0E+0011  0.000  13500.0  ! ME 165 CR
C8H18-1+R11C2H5=>C2H6+R31C8H17    6.0E+0011  0.000  13500.0  ! ME 166 CR
C8H18-1+R11C2H5=>C2H6+R32C8H17    1.0E+0011  0.000  9200.0  ! ME 167 CN
C8H18-1+R11C2H5=>C2H6+R33C8H17    2.0E+0011  0.000  11000.0  ! ME 168 CN
C7H16-1+R38C4H9=>C4H10+R26C7H15    1.0E+0011  0.000  12700.0  ! ME 169 CR
C7H16-1+R38C4H9=>C4H10+R27C7H15    3.0E+0011  0.000  15000.0  ! ME 170 CR
C7H16-1+R38C4H9=>C4H10+R28C7H15    2.0E+0011  0.000  12700.0  ! ME 171 CR
C7H16-1+R38C4H9=>C4H10+R29C7H15    2.0E+0011  0.000  12700.0  ! ME 172 CR
C8H18-1+R38C4H9=>C4H10+R30C8H17    4.5E+0011  0.000  15000.0  ! ME 173 CR
C8H18-1+R38C4H9=>C4H10+R31C8H17    3.0E+0011  0.000  15000.0  ! ME 174 CR
C8H18-1+R38C4H9=>C4H10+R32C8H17    5.0E+0010  0.000  11100.0  ! ME 175 CR
C8H18-1+R38C4H9=>C4H10+R33C8H17    1.0E+0011  0.000  12700.0  ! ME 176 CR

!   combinations :
R1H+R38C4H9=>C4H10    8.3E+0012  0.000  0.0  ! CO 177 KB
R1H+R43C3H7=>C3H8    8.3E+0012  0.000  0.0  ! CO 178 KB
R2OH+R38C4H9=>C4H10OL    5.7E+0012  0.000  0.0  ! CO 179 KB
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R2OH+R43C3H7=>C3H7OH    5.9E+0012  0.000  0.0  ! CO 180 KB
R3OOH+R38C4H9=>C4H10O2P    4.5E+0012  0.000  0.0  ! CO 181 KB
R3OOH+R43C3H7=>C3H8O2P    4.8E+0012  0.000  0.0  ! CO 182 KB
R4CH3+R38C4H9=>C5H12    1.5E+0013  0.000  0.0  ! CO 183 KB
R4CH3+R43C3H7=>C4H10    1.5E+0013  0.000  0.0  ! CO 184 KB
R5CHO+R38C4H9=>C5H10OA    4.9E+0012  0.000  0.0  ! CO 185 KB
R5CHO+R43C3H7=>C4H8OA    5.2E+0012  0.000  0.0  ! CO 186 KB
R6CH2OH+R38C4H9=>C5H12OL    4.8E+0012  0.000  0.0  ! CO 187 KB
R6CH2OH+R43C3H7=>C4H10OL    5.1E+0012  0.000  0.0  ! CO 188 KB
R11C2H5+R38C4H9=>C6H14    4.9E+0012  0.000  0.0  ! CO 189 KB
R11C2H5+R43C3H7=>C5H12    5.2E+0012  0.000  0.0  ! CO 190 KB
R38C4H9+R38C4H9=>C8H18    2.0E+0012  0.000  0.0  ! CO 191 KB
R38C4H9+R43C3H7=>C7H16    4.3E+0012  0.000  0.0  ! CO 192 KB
R43C3H7+R43C3H7=>C6H14    2.3E+0012  0.000  0.0  ! CO 193 KB

!   dismutations :

!    -------------------
!    SECONDARY MECHANISM
!    -------------------

!    Peroxide decomposition

! Hydroperoxide decomposition
C4H10O2P=>R2OH+R11C2H5+CH3CHO    1.5E+0016  0.000  43000.0  ! DHP 194
C3H8O2P=>R2OH+R11C2H5+HCHO    1.5E+0016  0.000  43000.0  ! DHP 195
C3H6O2PY=>R2OH+R1H+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 196
C4H8O2PY=>R2OH+R4CH3+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 197
C7H14O2PY=>R2OH+R20C4H9+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 198
C8H16O2PY=>R2OH+R35C5H11+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 199
C5H10O2PY=>R2OH+R11C2H5+C2H3CHOZ    1.5E+0016  0.000  43000.0  ! DHP 200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions
C3H8+R1H=>H2+R19C3H7    5.7E+0007  2.000  7700.0  ! MH 201
     DUPLICATE
C3H8+R1H=>H2+R19C3H7    9.0E+0006  2.000  5000.0  ! MH 202
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    5.4E+0006  2.000  450.0  ! MH 203
     DUPLICATE
C3H8+R2OH=>H2O+R19C3H7    2.6E+0006  2.000  -765.0  ! MH 204
     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    1.2E+0012  0.000  17000.0  ! MH 205
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     DUPLICATE
C3H8+R3OOH=>H2O2+R19C3H7    4.0E+0011  0.000  15500.0  ! MH 206
     DUPLICATE
C3H8+R4CH3=>CH4+R19C3H7    6.0E-0001  4.000  8200.0  ! MH 207
     DUPLICATE
C3H8+R4CH3=>CH4+R19C3H7    2.0E+0011  0.000  9600.0  ! MH 208
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    1.2E+0013  0.000  20000.0  ! MH 209
     DUPLICATE
C3H8+R8CH3OO=>CH3OOH+R19C3H7    3.0E+0012  0.000  17500.0  ! MH 210
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! MH 211
     DUPLICATE
C3H8+R11C2H5=>C2H6+R19C3H7    2.0E+0011  0.000  11000.0  ! MH 212
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    5.7E+0007  2.000  7700.0  ! MH 213
     DUPLICATE
C4H10+R1H=>H2+R20C4H9    1.8E+0007  2.000  5000.0  ! MH 214
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.4E+0006  2.000  450.0  ! MH 215
     DUPLICATE
C4H10+R2OH=>H2O+R20C4H9    5.2E+0006  2.000  -765.0  ! MH 216
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    1.2E+0012  0.000  17000.0  ! MH 217
     DUPLICATE
C4H10+R3OOH=>H2O2+R20C4H9    8.0E+0011  0.000  15500.0  ! MH 218
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    6.0E-0001  4.000  8200.0  ! MH 219
     DUPLICATE
C4H10+R4CH3=>CH4+R20C4H9    4.0E+0011  0.000  9600.0  ! MH 220
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    1.2E+0013  0.000  20000.0  ! MH 221
     DUPLICATE
C4H10+R8CH3OO=>CH3OOH+R20C4H9    6.0E+0012  0.000  17500.0  ! MH 222
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    6.0E+0011  0.000  13500.0  ! MH 223
     DUPLICATE
C4H10+R11C2H5=>C2H6+R20C4H9    4.0E+0011  0.000  11000.0  ! MH 224
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    5.7E+0007  2.000  7700.0  ! MH 225
     DUPLICATE
C5H12+R1H=>H2+R35C5H11    2.7E+0007  2.000  5000.0  ! MH 226
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    5.4E+0006  2.000  450.0  ! MH 227
     DUPLICATE
C5H12+R2OH=>H2O+R35C5H11    7.8E+0006  2.000  -765.0  ! MH 228
     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  17000.0  ! MH 229
     DUPLICATE
C5H12+R3OOH=>H2O2+R35C5H11    1.2E+0012  0.000  15500.0  ! MH 230
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E-0001  4.000  8200.0  ! MH 231
     DUPLICATE
C5H12+R4CH3=>CH4+R35C5H11    6.0E+0011  0.000  9600.0  ! MH 232
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     DUPLICATE
C5H12+R8CH3OO=>CH3OOH+R35C5H11    1.2E+0013  0.000  20000.0  ! MH 233
     DUPLICATE
C5H12+R8CH3OO=>CH3OOH+R35C5H11    9.0E+0012  0.000  17500.0  ! MH 234
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  13500.0  ! MH 235
     DUPLICATE
C5H12+R11C2H5=>C2H6+R35C5H11    6.0E+0011  0.000  11000.0  ! MH 236
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    5.7E+0007  2.000  7700.0  ! MH 237
     DUPLICATE
C6H14+R1H=>H2+R41C6H13    3.6E+0007  2.000  5000.0  ! MH 238
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    5.4E+0006  2.000  450.0  ! MH 239
     DUPLICATE
C6H14+R2OH=>H2O+R41C6H13    1.0E+0007  2.000  -765.0  ! MH 240
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.2E+0012  0.000  17000.0  ! MH 241
     DUPLICATE
C6H14+R3OOH=>H2O2+R41C6H13    1.6E+0012  0.000  15500.0  ! MH 242
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    6.0E-0001  4.000  8200.0  ! MH 243
     DUPLICATE
C6H14+R4CH3=>CH4+R41C6H13    8.0E+0011  0.000  9600.0  ! MH 244
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  20000.0  ! MH 245
     DUPLICATE
C6H14+R8CH3OO=>CH3OOH+R41C6H13    1.2E+0013  0.000  17500.0  ! MH 246
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    6.0E+0011  0.000  13500.0  ! MH 247
     DUPLICATE
C6H14+R11C2H5=>C2H6+R41C6H13    8.0E+0011  0.000  11000.0  ! MH 248
     DUPLICATE

! O-ring decomposition
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 249
     DUPLICATE
C3H6OE#3+R1H=>H2+R4CH3+CH2COZ    1.3E+0007  2.000  5000.0  ! DE# 250
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 251
     DUPLICATE
C3H6OE#3+R2OH=>H2O+R4CH3+CH2COZ    3.9E+0006  2.000  -765.0  ! DE# 252
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  17000.0  ! DE# 253
     DUPLICATE
C3H6OE#3+R3OOH=>H2O2+R4CH3+CH2COZ    6.0E+0011  0.000  15500.0  ! DE# 254
     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 255
     DUPLICATE
C3H6OE#3+R4CH3=>CH4+R4CH3+CH2COZ    3.0E+0011  0.000  9600.0  ! DE# 256
     DUPLICATE
C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    6.0E+0012  0.000  20000.0  ! DE#
257
     DUPLICATE
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C3H6OE#3+R8CH3OO=>CH3OOH+R4CH3+CH2COZ    4.5E+0012  0.000  17500.0  ! DE#
258
     DUPLICATE
C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
259
     DUPLICATE
C3H6OE#3+R11C2H5=>C2H6+R4CH3+CH2COZ    3.0E+0011  0.000  11000.0  ! DE#
260
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 261
     DUPLICATE
C4H8OE#3+R1H=>H2+R11C2H5+CH2COZ    2.3E+0007  2.000  5000.0  ! DE# 262
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 263
     DUPLICATE
C4H8OE#3+R2OH=>H2O+R11C2H5+CH2COZ    6.5E+0006  2.000  -765.0  ! DE# 264
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
265
     DUPLICATE
C4H8OE#3+R3OOH=>H2O2+R11C2H5+CH2COZ    1.0E+0012  0.000  15500.0  ! DE#
266
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    3.0E-0001  4.000  8200.0  ! DE# 267
     DUPLICATE
C4H8OE#3+R4CH3=>CH4+R11C2H5+CH2COZ    5.0E+0011  0.000  9600.0  ! DE# 268
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 269
     DUPLICATE
C4H8OE#3+R8CH3OO=>CH3OOH+R11C2H5+CH2COZ    7.5E+0012  0.000  17500.0  !
DE# 270
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    3.0E+0011  0.000  13500.0  ! DE#
271
     DUPLICATE
C4H8OE#3+R11C2H5=>C2H6+R11C2H5+CH2COZ    5.0E+0011  0.000  11000.0  ! DE#
272
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    2.9E+0007  2.000  7700.0  ! DE# 273
     DUPLICATE
C5H10OE#3+R1H=>H2+R19C3H7+CH2COZ    3.2E+0007  2.000  5000.0  ! DE# 274
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    2.7E+0006  2.000  450.0  ! DE# 275
     DUPLICATE
C5H10OE#3+R2OH=>H2O+R19C3H7+CH2COZ    9.1E+0006  2.000  -765.0  ! DE# 276
     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    6.0E+0011  0.000  17000.0  ! DE#
277
     DUPLICATE
C5H10OE#3+R3OOH=>H2O2+R19C3H7+CH2COZ    1.4E+0012  0.000  15500.0  ! DE#
278
     DUPLICATE
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C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    3.0E-0001  4.000  8200.0  ! DE#
279
     DUPLICATE
C5H10OE#3+R4CH3=>CH4+R19C3H7+CH2COZ    7.0E+0011  0.000  9600.0  ! DE#
280
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    6.0E+0012  0.000  20000.0  !
DE# 281
     DUPLICATE
C5H10OE#3+R8CH3OO=>CH3OOH+R19C3H7+CH2COZ    1.0E+0013  0.000  17500.0  !
DE# 282
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    3.0E+0011  0.000  13500.0  !
DE# 283
     DUPLICATE
C5H10OE#3+R11C2H5=>C2H6+R19C3H7+CH2COZ    7.0E+0011  0.000  11000.0  !
DE# 284
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 285
     DUPLICATE
C7H14OE#3+R1H=>H2+R20C4H9+C2H3CHOZ    5.0E+0007  2.000  5000.0  ! DE# 286
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
287
     DUPLICATE
C7H14OE#3+R2OH=>H2O+R20C4H9+C2H3CHOZ    1.4E+0007  2.000  -765.0  ! DE#
288
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 289
     DUPLICATE
C7H14OE#3+R3OOH=>H2O2+R20C4H9+C2H3CHOZ    2.2E+0012  0.000  15500.0  !
DE# 290
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
291
     DUPLICATE
C7H14OE#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  9600.0  ! DE#
292
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 293
     DUPLICATE
C7H14OE#3+R8CH3OO=>CH3OOH+R20C4H9+C2H3CHOZ    1.7E+0013  0.000
17500.0  ! DE# 294
     DUPLICATE
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 295
     DUPLICATE
C7H14OE#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ    1.1E+0012  0.000  11000.0  !
DE# 296
     DUPLICATE
C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    2.9E+0007  2.000  7700.0  ! DE# 297
     DUPLICATE
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C6H12OE#3+R1H=>H2+R19C3H7+C2H3CHOZ    4.1E+0007  2.000  5000.0  ! DE# 298
     DUPLICATE
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    2.7E+0006  2.000  450.0  ! DE#
299
     DUPLICATE
C6H12OE#3+R2OH=>H2O+R19C3H7+C2H3CHOZ    1.1E+0007  2.000  -765.0  ! DE#
300
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    6.0E+0011  0.000  17000.0  !
DE# 301
     DUPLICATE
C6H12OE#3+R3OOH=>H2O2+R19C3H7+C2H3CHOZ    1.8E+0012  0.000  15500.0  !
DE# 302
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    3.0E-0001  4.000  8200.0  ! DE#
303
     DUPLICATE
C6H12OE#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  9600.0  ! DE#
304
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    6.0E+0012  0.000
20000.0  ! DE# 305
     DUPLICATE
C6H12OE#3+R8CH3OO=>CH3OOH+R19C3H7+C2H3CHOZ    1.3E+0013  0.000
17500.0  ! DE# 306
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    3.0E+0011  0.000  13500.0  !
DE# 307
     DUPLICATE
C6H12OE#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ    9.0E+0011  0.000  11000.0  !
DE# 308
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE# 309
     DUPLICATE
C8H16OE#3+R1H=>H2+R20C4H9+C4H6OKZ    5.9E+0007  2.000  5000.0  ! DE# 310
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE# 311
     DUPLICATE
C8H16OE#3+R2OH=>H2O+R20C4H9+C4H6OKZ    1.7E+0007  2.000  -765.0  ! DE#
312
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    6.0E+0011  0.000  17000.0  ! DE#
313
     DUPLICATE
C8H16OE#3+R3OOH=>H2O2+R20C4H9+C4H6OKZ    2.6E+0012  0.000  15500.0  ! DE#
314
     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
315
     DUPLICATE
C8H16OE#3+R4CH3=>CH4+R20C4H9+C4H6OKZ    1.3E+0012  0.000  9600.0  ! DE#
316
     DUPLICATE
```

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C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    6.0E+0012  0.000  20000.0  !
DE# 317
     DUPLICATE
C8H16OE#3+R8CH3OO=>CH3OOH+R20C4H9+C4H6OKZ    2.0E+0013  0.000  17500.0  !
DE# 318
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 319
     DUPLICATE
C8H16OE#3+R11C2H5=>C2H6+R20C4H9+C4H6OKZ    1.3E+0012  0.000  11000.0  !
DE# 320
     DUPLICATE
!C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    2.9E+0007  2.000  7700.0  ! DE#
321
     DUPLICATE
!C9H18OE#3+R1H=>H2+R35C5H11+C4H6OKZ    6.8E+0007  2.000  5000.0  ! DE#
322
     DUPLICATE
!C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.7E+0006  2.000  450.0  ! DE#
323
     DUPLICATE
!C9H18OE#3+R2OH=>H2O+R35C5H11+C4H6OKZ    2.0E+0007  2.000  -765.0  ! DE#
324
     DUPLICATE
!C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    6.0E+0011  0.000  17000.0  !
DE# 325
     DUPLICATE
!C9H18OE#3+R3OOH=>H2O2+R35C5H11+C4H6OKZ    3.0E+0012  0.000  15500.0  !
DE# 326
     DUPLICATE
!C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    3.0E-0001  4.000  8200.0  ! DE#
327
     DUPLICATE
!C9H18OE#3+R4CH3=>CH4+R35C5H11+C4H6OKZ    1.5E+0012  0.000  9600.0  ! DE#
328
     DUPLICATE
!C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    6.0E+0012  0.000  20000.0
! DE# 329
     DUPLICATE
!C9H18OE#3+R8CH3OO=>CH3OOH+R35C5H11+C4H6OKZ    2.3E+0013  0.000  17500.0
! DE# 330
     DUPLICATE
!C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    3.0E+0011  0.000  13500.0  !
DE# 331
     DUPLICATE
!C9H18OE#3+R11C2H5=>C2H6+R35C5H11+C4H6OKZ    1.5E+0012  0.000  11000.0  !
DE# 332
     DUPLICATE
!C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
333
     DUPLICATE
!C10H20OE#3+R1H=>H2+R35C5H11+C5H8OKZ    7.7E+0007  2.000  5000.0  ! DE#
334
     DUPLICATE
```

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!C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
335
     DUPLICATE
!C10H20OE#3+R2OH=>H2O+R35C5H11+C5H8OKZ    2.2E+0007  2.000  -765.0  ! DE#
336
     DUPLICATE
!C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 337
     DUPLICATE
!C10H20OE#3+R3OOH=>H2O2+R35C5H11+C5H8OKZ    3.4E+0012  0.000  15500.0  !
DE# 338
     DUPLICATE
!C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    3.0E-0001  4.000  8200.0  !
DE# 339
     DUPLICATE
!C10H20OE#3+R4CH3=>CH4+R35C5H11+C5H8OKZ    1.7E+0012  0.000  9600.0  !
DE# 340
     DUPLICATE
!C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 341
     DUPLICATE
!C10H20OE#3+R8CH3OO=>CH3OOH+R35C5H11+C5H8OKZ    2.6E+0013  0.000  17500.0
! DE# 342
     DUPLICATE
!C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    3.0E+0011  0.000
13500.0  ! DE# 343
     DUPLICATE
!C10H20OE#3+R11C2H5=>C2H6+R35C5H11+C5H8OKZ    1.7E+0012  0.000
11000.0  ! DE# 344
     DUPLICATE
!C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
345
     DUPLICATE
!C13H26OE#3+R1H=>H2+R26C7H15+C6H10OKZ    1.0E+0008  2.000  5000.0  ! DE#
346
     DUPLICATE
!C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
347
     DUPLICATE
!C13H26OE#3+R2OH=>H2O+R26C7H15+C6H10OKZ    3.0E+0007  2.000  -765.0  !
DE# 348
     DUPLICATE
!C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 349
     DUPLICATE
!C13H26OE#3+R3OOH=>H2O2+R26C7H15+C6H10OKZ    4.6E+0012  0.000  15500.0  !
DE# 350
     DUPLICATE
!C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 351
     DUPLICATE
!C13H26OE#3+R4CH3=>CH4+R26C7H15+C6H10OKZ    2.3E+0012  0.000  9600.0  !
DE# 352
     DUPLICATE
```

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!C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    6.0E+0012  0.000
20000.0  ! DE# 353
     DUPLICATE
!C13H26OE#3+R8CH3OO=>CH3OOH+R26C7H15+C6H10OKZ    3.5E+0013  0.000
17500.0  ! DE# 354
     DUPLICATE
!C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    3.0E+0011  0.000  13500.0
! DE# 355
     DUPLICATE
!C13H26OE#3+R11C2H5=>C2H6+R26C7H15+C6H10OKZ    2.3E+0012  0.000  11000.0
! DE# 356
     DUPLICATE
!C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    2.9E+0007  2.000  7700.0  ! DE#
357
     DUPLICATE
!C12H24OE#3+R1H=>H2+R41C6H13+C6H10OKZ    9.5E+0007  2.000  5000.0  ! DE#
358
     DUPLICATE
!C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0006  2.000  450.0  ! DE#
359
     DUPLICATE
!C12H24OE#3+R2OH=>H2O+R41C6H13+C6H10OKZ    2.7E+0007  2.000  -765.0  !
DE# 360
     DUPLICATE
!C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    6.0E+0011  0.000  17000.0  !
DE# 361
     DUPLICATE
!C12H24OE#3+R3OOH=>H2O2+R41C6H13+C6H10OKZ    4.2E+0012  0.000  15500.0  !
DE# 362
     DUPLICATE
!C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    3.0E-0001  4.000  8200.0  !
DE# 363
     DUPLICATE
!C12H24OE#3+R4CH3=>CH4+R41C6H13+C6H10OKZ    2.1E+0012  0.000  9600.0  !
DE# 364
     DUPLICATE
!C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    6.0E+0012  0.000
20000.0  ! DE# 365
     DUPLICATE
!C12H24OE#3+R8CH3OO=>CH3OOH+R41C6H13+C6H10OKZ    3.2E+0013  0.000
17500.0  ! DE# 366
     DUPLICATE
!C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    3.0E+0011  0.000  13500.0
! DE# 367
     DUPLICATE
!C12H24OE#3+R11C2H5=>C2H6+R41C6H13+C6H10OKZ    2.1E+0012  0.000  11000.0
! DE# 368
     DUPLICATE
!C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    2.9E+0007  2.000  7700.0  ! DE#
369
     DUPLICATE
!C11H22OE#3+R1H=>H2+R41C6H13+C5H8OKZ    8.6E+0007  2.000  5000.0  ! DE#
370
     DUPLICATE
```

```
!C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.7E+0006  2.000  450.0  ! DE#
371
     DUPLICATE
!C11H22OE#3+R2OH=>H2O+R41C6H13+C5H8OKZ    2.5E+0007  2.000  -765.0  ! DE#
372
     DUPLICATE
!C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    6.0E+0011  0.000  17000.0  !
DE# 373
     DUPLICATE
!C11H22OE#3+R3OOH=>H2O2+R41C6H13+C5H8OKZ    3.8E+0012  0.000  15500.0  !
DE# 374
     DUPLICATE
!C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    3.0E-0001  4.000  8200.0  !
DE# 375
     DUPLICATE
!C11H22OE#3+R4CH3=>CH4+R41C6H13+C5H8OKZ    1.9E+0012  0.000  9600.0  !
DE# 376
     DUPLICATE
!C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    6.0E+0012  0.000  20000.0
! DE# 377
     DUPLICATE
!C11H22OE#3+R8CH3OO=>CH3OOH+R41C6H13+C5H8OKZ    2.9E+0013  0.000  17500.0
! DE# 378
     DUPLICATE
!C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    3.0E+0011  0.000
13500.0  ! DE# 379
     DUPLICATE
!C11H22OE#3+R11C2H5=>C2H6+R41C6H13+C5H8OKZ    1.9E+0012  0.000
11000.0  ! DE# 380
     DUPLICATE
!C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    2.9E+0007  2.000  7700.0  ! DE#
381
     DUPLICATE
!C14H28OE#3+R1H=>H2+R26C7H15+C7H12OKZ    1.1E+0008  2.000  5000.0  ! DE#
382
     DUPLICATE
!C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    2.7E+0006  2.000  450.0  ! DE#
383
     DUPLICATE
!C14H28OE#3+R2OH=>H2O+R26C7H15+C7H12OKZ    3.3E+0007  2.000  -765.0  !
DE# 384
     DUPLICATE
!C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    6.0E+0011  0.000  17000.0  !
DE# 385
     DUPLICATE
!C14H28OE#3+R3OOH=>H2O2+R26C7H15+C7H12OKZ    5.0E+0012  0.000  15500.0  !
DE# 386
     DUPLICATE
!C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    3.0E-0001  4.000  8200.0  !
DE# 387
     DUPLICATE
!C14H28OE#3+R4CH3=>CH4+R26C7H15+C7H12OKZ    2.5E+0012  0.000  9600.0  !
DE# 388
     DUPLICATE
```

```
!C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    6.0E+0012  0.000
20000.0  ! DE# 389
     DUPLICATE
!C14H28OE#3+R8CH3OO=>CH3OOH+R26C7H15+C7H12OKZ    3.8E+0013  0.000
17500.0  ! DE# 390
     DUPLICATE
!C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    3.0E+0011  0.000  13500.0
! DE# 391
     DUPLICATE
!C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H12OKZ    2.5E+0012  0.000  11000.0
! DE# 392
     DUPLICATE


! Metatheses of oxetanes, furanes and pyranes

! decompositions of cyclo-ether radicals

! Addition of oxygen on cyclo-ether radicals
!    O2 elimination
!    Isomerization
!    Cylo-ether keto-hydroperoxide ester formation
!    Decomposition of cylo-ether keto-hydroperoxide ester

! Isomerization of peroxy-radicals

!Addition of oxygen on cyclo-peroxy radicals

! Formation of cyclo-ether ketohydroperoxydes

! Decomposition of cyclo-ether ketohydroperoxydes

! Olefin reactions
!  addition of H and CH3 on olefins
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  1560.0  ! ADZ 393
     DUPLICATE
C3H6Y+R1H=>R19C3H7    1.3E+0013  0.000  3260.0  ! ADZ 394
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  1560.0  ! ADZ 395
     DUPLICATE
C4H8Y+R1H=>R20C4H9    1.3E+0013  0.000  3260.0  ! ADZ 396
     DUPLICATE
C4H8Y+R4CH3=>C3H6Y+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 397
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 398
     DUPLICATE
C5H10Z+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 399
     DUPLICATE
C5H10Z+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 400
C5H10Z+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 401
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 402
     DUPLICATE
C7H14Z+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 403
     DUPLICATE
C7H14Z+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 404
```

```
C7H14Z+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 405
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  1560.0  ! ADZ 406
     DUPLICATE
C6H12Z+R1H=>R41C6H13    1.3E+0013  0.000  3260.0  ! ADZ 407
     DUPLICATE
C6H12Z+R4CH3=>C4H8Y+R19C3H7    1.7E+0011  0.000  7400.0  ! ADZ 408
C6H12Z+R4CH3=>C3H6Y+R20C4H9    9.6E+0010  0.000  8000.0  ! ADZ 409
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  1560.0  ! ADZ 410
     DUPLICATE
C7H14Y+R1H=>R26C7H15    1.3E+0013  0.000  3260.0  ! ADZ 411
     DUPLICATE
C7H14Y+R4CH3=>C4H8Y+R20C4H9    1.7E+0011  0.000  7400.0  ! ADZ 412
C7H14Y+R4CH3=>C3H6Y+R35C5H11    9.6E+0010  0.000  8000.0  ! ADZ 413
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 414
     DUPLICATE
C8H16Y+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 415
     DUPLICATE
C8H16Y+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 416
C8H16Y+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 417
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  1560.0  ! ADZ 418
     DUPLICATE
C8H16Z+R1H=>R30C8H17    1.3E+0013  0.000  3260.0  ! ADZ 419
     DUPLICATE
C8H16Z+R4CH3=>C4H8Y+R35C5H11    1.7E+0011  0.000  7400.0  ! ADZ 420
C8H16Z+R4CH3=>C3H6Y+R41C6H13    9.6E+0010  0.000  8000.0  ! ADZ 421
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  1560.0  ! ADZ 422
     DUPLICATE
C5H10Y+R1H=>R35C5H11    1.3E+0013  0.000  3260.0  ! ADZ 423
     DUPLICATE
C5H10Y+R4CH3=>C4H8Y+R11C2H5    1.7E+0011  0.000  7400.0  ! ADZ 424
C5H10Y+R4CH3=>C3H6Y+R19C3H7    9.6E+0010  0.000  8000.0  ! ADZ 425
!C9H18Z+R4CH3=>C4H8Y+R41C6H13    1.7E+0011  0.000  7400.0  ! ADZ 426
!C9H18Z+R4CH3=>C3H6Y+R26C7H15    9.6E+0010  0.000  8000.0  ! ADZ 427
!C10H20Z+R4CH3=>C4H8Y+R26C7H15    1.7E+0011  0.000  7400.0  ! ADZ 428
!C10H20Z+R4CH3=>C3H6Y+R30C8H17    9.6E+0010  0.000  8000.0  ! ADZ 429
!C11H22Z+R4CH3=>C4H8Y+R30C8H17    1.7E+0011  0.000  7400.0  ! ADZ 430
!C9H18Z+R1H=>4C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 431
!C10H20Z+R1H=>4C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 432
!C13H26Z+R1H=>6C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 433
!C12H24Z+R1H=>5C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 434
!C11H22Z+R1H=>5C2H4Z+R4CH3    9.6E+0010  0.000  8000.0  ! ADZ 435
!C14H28Z+R1H=>6C2H4Z+R11C2H5    9.6E+0010  0.000  8000.0  ! ADZ 436

!  addition of OH on olefins
C3H6Y+R2OH=>R4CH3+CH3CHO    1.4E+0012  0.000  -1040.0  ! ADZ 437
C3H6Y+R2OH=>R11C2H5+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 438
C4H8Y+R2OH=>R4CH3+C2H5CHO    1.4E+0012  0.000  -1040.0  ! ADZ 439
C4H8Y+R2OH=>R19C3H7+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 440
C5H10Z+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 441
C5H10Z+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 442
C7H14Z+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 443
C7H14Z+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 444
C6H12Z+R2OH=>R4CH3+C5H10OA    1.4E+0012  0.000  -1040.0  ! ADZ 445
C6H12Z+R2OH=>R35C5H11+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 446
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C7H14Y+R2OH=>R4CH3+C6H12OA    1.4E+0012  0.000  -1040.0  ! ADZ 447
C7H14Y+R2OH=>R41C6H13+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 448
C8H16Y+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 449
C8H16Y+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 450
C8H16Z+R2OH=>R4CH3+C7H14OA    1.4E+0012  0.000  -1040.0  ! ADZ 451
C8H16Z+R2OH=>R26C7H15+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 452
C5H10Y+R2OH=>R4CH3+C4H8OA    1.4E+0012  0.000  -1040.0  ! ADZ 453
C5H10Y+R2OH=>R20C4H9+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 454
!C9H18Z+R2OH=>R4CH3+C8H16OA    1.4E+0012  0.000  -1040.0  ! ADZ 455
!C9H18Z+R2OH=>R30C8H17+HCHO    1.4E+0012  0.000  -1040.0  ! ADZ 456
!C10H20Z+R2OH=>R4CH3+C9H18OA    1.4E+0012  0.000  -1040.0  ! ADZ 457
!C13H26Z+R2OH=>R4CH3+C12H24OA    1.4E+0012  0.000  -1040.0  ! ADZ 458
!C12H24Z+R2OH=>R4CH3+C11H22OA    1.4E+0012  0.000  -1040.0  ! ADZ 459
!C11H22Z+R2OH=>R4CH3+C10H20OA    1.4E+0012  0.000  -1040.0  ! ADZ 460
!C14H28Z+R2OH=>R4CH3+C13H26OA    1.4E+0012  0.000  -1040.0  ! ADZ 461

!C10H20Z+R2OH=>HCHO+R4CH3+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 462
!C13H26Z+R2OH=>HCHO+R11C2H5+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH
463
!C12H24Z+R2OH=>HCHO+R4CH3+5C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 464
!C11H22Z+R2OH=>HCHO+R11C2H5+4C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH
465
!C14H28Z+R2OH=>HCHO+R4CH3+6C2H4Z    1.4E+0012  0.000  -1040.0  ! FOH 466

!  addition of O on olefins
C3H6Y+B1O=>CH2COZ+R1H+R4CH3    1.2E+0005  2.560  -1130.0  ! AOZ 467
C4H8Y+B1O=>CH2COZ+R1H+R11C2H5    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Z+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Z+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C6H12Z+B1O=>CH2COZ+R1H+R20C4H9    1.2E+0005  2.560  -1130.0  ! AOZ 467
C7H14Y+B1O=>CH2COZ+R1H+R35C5H11    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Y+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C8H16Z+B1O=>CH2COZ+R1H+R41C6H13    1.2E+0005  2.560  -1130.0  ! AOZ 467
C5H10Y+B1O=>CH2COZ+R1H+R19C3H7    1.2E+0005  2.560  -1130.0  ! AOZ 467
!C9H18Z+B1O=>CH2COZ+R1H+R26C7H15    1.2E+0005  2.560  -1130.0  ! AOZ 467
!C10H20Z+B1O=>CH2COZ+R1H+R30C8H17    1.2E+0005  2.560  -1130.0  ! AOZ 467
!C13H26Z+B1O=>CH2COZ+R4CH3+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C12H24Z+B1O=>CH2COZ+R11C2H5+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467
!C11H22Z+B1O=>CH2COZ+R4CH3+R1H+4C2H4Z    7.8E+0013  0.000  5200.0  ! AOZ
467
!C14H28Z+B1O=>CH2COZ+R11C2H5+R1H+5C2H4Z    7.8E+0013  0.000  5200.0  !
AOZ 467

! retroene reactions
C5H10Z=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 467
C7H14Z=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 468
C6H12Z=>C3H6Y+C3H6Y    8.0E+0012  0.000  56500.0  ! RTZ 469
C7H14Y=>C3H6Y+C4H8Y    8.0E+0012  0.000  56500.0  ! RTZ 470
C8H16Y=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 471
C8H16Z=>C3H6Y+C5H10Z    8.0E+0012  0.000  56500.0  ! RTZ 472
C5H10Y=>C3H6Y+C2H4Z    8.0E+0012  0.000  56500.0  ! RTZ 473
!C9H18Z=>C3H6Y+C6H12Z    8.0E+0012  0.000  56500.0  ! RTZ 474
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!C10H20Z=>C3H6Y+C7H14Z    8.0E+0012  0.000  56500.0  ! RTZ 475
!C13H26Z=>C3H6Y+C10H20Z    8.0E+0012  0.000  56500.0  ! RTZ 476
!C12H24Z=>C3H6Y+C9H18Z    8.0E+0012  0.000  56500.0  ! RTZ 477
!C11H22Z=>C3H6Y+C8H16Z    8.0E+0012  0.000  56500.0  ! RTZ 478
!C14H28Z=>C3H6Y+C11H22Z    8.0E+0012  0.000  56500.0  ! RTZ 479

!  addition of OOH on olefins
C3H6Y+R3OOH=>R2OH+C3H6OE#3    1.0E+0012  0.000  14200.0  ! ADZ 480
C4H8Y+R3OOH=>R2OH+C4H8OE#3    1.0E+0012  0.000  14200.0  ! ADZ 481
C5H10Z+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 482
C7H14Z+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 483
C6H12Z+R3OOH=>R2OH+C6H12OE#3    1.0E+0012  0.000  14200.0  ! ADZ 484
C7H14Y+R3OOH=>R2OH+C7H14OE#3    1.0E+0012  0.000  14200.0  ! ADZ 485
C8H16Y+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 486
C8H16Z+R3OOH=>R2OH+C8H16OE#3    1.0E+0012  0.000  14200.0  ! ADZ 487
C5H10Y+R3OOH=>R2OH+C5H10OE#3    1.0E+0012  0.000  14200.0  ! ADZ 488
!C9H18Z+R3OOH=>R2OH+C9H18OE#3    1.0E+0012  0.000  14200.0  ! ADZ 489
!C10H20Z+R3OOH=>R2OH+C10H20OE#3    1.0E+0012  0.000  14200.0  ! ADZ 490
!C13H26Z+R3OOH=>R2OH+C13H26OE#3    1.0E+0012  0.000  14200.0  ! ADZ 491
!C12H24Z+R3OOH=>R2OH+C12H24OE#3    1.0E+0012  0.000  14200.0  ! ADZ 492
!C11H22Z+R3OOH=>R2OH+C11H22OE#3    1.0E+0012  0.000  14200.0  ! ADZ 493
!C14H28Z+R3OOH=>R2OH+C14H28OE#3    1.0E+0012  0.000  14200.0  ! ADZ 494

!   olefin to dienes
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    5.4E+0004  2.500  -1900.0  ! MZ 495
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    2.9E+0007  2.000  7700.0  ! MZ 496
     DUPLICATE
C5H10Z+R1H=>H2+C4H6Z2+R4CH3    9.0E+0006  2.000  5000.0  ! MZ 497
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    3.0E+0006  2.000  -1520.0  ! MZ 498
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.7E+0006  2.000  450.0  ! MZ 499
     DUPLICATE
C5H10Z+R2OH=>H2O+C4H6Z2+R4CH3    2.6E+0006  2.000  -765.0  ! MZ 500
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.4E+0003  2.600  12400.0  ! MZ 501
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    6.0E+0011  0.000  17000.0  ! MZ 502
     DUPLICATE
C5H10Z+R3OOH=>H2O2+C4H6Z2+R4CH3    4.0E+0011  0.000  15500.0  ! MZ 503
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    1.0E+0011  0.000  7300.0  ! MZ 504
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    3.0E-0001  4.000  8200.0  ! MZ 505
     DUPLICATE
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3    2.0E+0011  0.000  9600.0  ! MZ 506
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    1.0E+0012  0.000  14550.0  ! MZ
507
     DUPLICATE
C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    6.0E+0012  0.000  20000.0  ! MZ
508
     DUPLICATE
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C5H10Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3    3.0E+0012  0.000  17500.0  ! MZ
509
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    1.5E+0000  3.500  4140.0  ! MZ 510
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    3.0E+0011  0.000  13500.0  ! MZ 511
     DUPLICATE
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3    2.0E+0011  0.000  11000.0  ! MZ 512
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    5.4E+0004  2.500  -1900.0  ! MZ 513
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.9E+0007  2.000  7700.0  ! MZ 514
     DUPLICATE
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7    2.7E+0007  2.000  5000.0  ! MZ 515
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    3.0E+0006  2.000  -1520.0  ! MZ 516
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    2.7E+0006  2.000  450.0  ! MZ 517
     DUPLICATE
C7H14Z+R2OH=>H2O+C4H6Z2+R19C3H7    7.8E+0006  2.000  -765.0  ! MZ 518
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.4E+0003  2.600  12400.0  ! MZ 519
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    6.0E+0011  0.000  17000.0  ! MZ 520
     DUPLICATE
C7H14Z+R3OOH=>H2O2+C4H6Z2+R19C3H7    1.2E+0012  0.000  15500.0  ! MZ 521
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    1.0E+0011  0.000  7300.0  ! MZ 522
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    3.0E-0001  4.000  8200.0  ! MZ 523
     DUPLICATE
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7    6.0E+0011  0.000  9600.0  ! MZ 524
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    1.0E+0012  0.000  14550.0  ! MZ
525
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    6.0E+0012  0.000  20000.0  ! MZ
526
     DUPLICATE
C7H14Z+R8CH3OO=>CH3OOH+C4H6Z2+R19C3H7    9.0E+0012  0.000  17500.0  ! MZ
527
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    1.5E+0000  3.500  4140.0  ! MZ 528
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    3.0E+0011  0.000  13500.0  ! MZ
529
     DUPLICATE
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7    6.0E+0011  0.000  11000.0  ! MZ
530
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    5.4E+0004  2.500  -1900.0  ! MZ 531
     DUPLICATE
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    2.9E+0007  2.000  7700.0  ! MZ 532
     DUPLICATE
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C6H12Z+R1H=>H2+C4H6Z2+R11C2H5    1.8E+0007  2.000  5000.0  ! MZ 533
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    3.0E+0006  2.000  -1520.0  ! MZ 534
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    2.7E+0006  2.000  450.0  ! MZ 535
     DUPLICATE
C6H12Z+R2OH=>H2O+C4H6Z2+R11C2H5    5.2E+0006  2.000  -765.0  ! MZ 536
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.4E+0003  2.600  12400.0  ! MZ 537
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    6.0E+0011  0.000  17000.0  ! MZ 538
     DUPLICATE
C6H12Z+R3OOH=>H2O2+C4H6Z2+R11C2H5    8.0E+0011  0.000  15500.0  ! MZ 539
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    1.0E+0011  0.000  7300.0  ! MZ 540
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    3.0E-0001  4.000  8200.0  ! MZ 541
     DUPLICATE
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5    4.0E+0011  0.000  9600.0  ! MZ 542
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    1.0E+0012  0.000  14550.0  ! MZ
543
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  20000.0  ! MZ
544
     DUPLICATE
C6H12Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5    6.0E+0012  0.000  17500.0  ! MZ
545
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    1.5E+0000  3.500  4140.0  ! MZ 546
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    3.0E+0011  0.000  13500.0  ! MZ
547
     DUPLICATE
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5    4.0E+0011  0.000  11000.0  ! MZ
548
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    5.4E+0004  2.500  -1900.0  ! MZ 549
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    2.9E+0007  2.000  7700.0  ! MZ 550
     DUPLICATE
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9    3.6E+0007  2.000  5000.0  ! MZ 551
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    3.0E+0006  2.000  -1520.0  ! MZ 552
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    2.7E+0006  2.000  450.0  ! MZ 553
     DUPLICATE
C8H16Z+R2OH=>H2O+C4H6Z2+R20C4H9    1.0E+0007  2.000  -765.0  ! MZ 554
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.4E+0003  2.600  12400.0  ! MZ 555
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    6.0E+0011  0.000  17000.0  ! MZ 556
     DUPLICATE
C8H16Z+R3OOH=>H2O2+C4H6Z2+R20C4H9    1.6E+0012  0.000  15500.0  ! MZ 557
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     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    1.0E+0011  0.000  7300.0  ! MZ 558
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    3.0E-0001  4.000  8200.0  ! MZ 559
     DUPLICATE
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9    8.0E+0011  0.000  9600.0  ! MZ 560
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.0E+0012  0.000  14550.0  ! MZ
561
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    6.0E+0012  0.000  20000.0  ! MZ
562
     DUPLICATE
C8H16Z+R8CH3OO=>CH3OOH+C4H6Z2+R20C4H9    1.2E+0013  0.000  17500.0  ! MZ
563
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    1.5E+0000  3.500  4140.0  ! MZ 564
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    3.0E+0011  0.000  13500.0  ! MZ
565
     DUPLICATE
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9    8.0E+0011  0.000  11000.0  ! MZ
566
     DUPLICATE
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    5.4E+0004  2.500  -1900.0  ! MZ 567
     DUPLICATE
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    2.9E+0007  2.000  7700.0  ! MZ 568
     DUPLICATE
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11    4.5E+0007  2.000  5000.0  ! MZ 569
     DUPLICATE
!C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    3.0E+0006  2.000  -1520.0  ! MZ 570
     DUPLICATE
!C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    2.7E+0006  2.000  450.0  ! MZ 571
     DUPLICATE
!C9H18Z+R2OH=>H2O+C4H6Z2+R35C5H11    1.3E+0007  2.000  -765.0  ! MZ 572
     DUPLICATE
!C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.4E+0003  2.600  12400.0  ! MZ
573
     DUPLICATE
!C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    6.0E+0011  0.000  17000.0  ! MZ
574
     DUPLICATE
!C9H18Z+R3OOH=>H2O2+C4H6Z2+R35C5H11    2.0E+0012  0.000  15500.0  ! MZ
575
     DUPLICATE
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0011  0.000  7300.0  ! MZ 576
     DUPLICATE
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    3.0E-0001  4.000  8200.0  ! MZ 577
     DUPLICATE
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11    1.0E+0012  0.000  9600.0  ! MZ 578
     DUPLICATE
!C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.0E+0012  0.000  14550.0  !
MZ 579
     DUPLICATE
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!C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    6.0E+0012  0.000  20000.0  !
MZ 580
     DUPLICATE
!C9H18Z+R8CH3OO=>CH3OOH+C4H6Z2+R35C5H11    1.5E+0013  0.000  17500.0  !
MZ 581
     DUPLICATE
!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.5E+0000  3.500  4140.0  ! MZ
582
     DUPLICATE
!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    3.0E+0011  0.000  13500.0  ! MZ
583
     DUPLICATE
!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11    1.0E+0012  0.000  11000.0  ! MZ
584
     DUPLICATE
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0004  2.500  -1900.0  ! MZ 585
     DUPLICATE
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    2.9E+0007  2.000  7700.0  ! MZ 586
     DUPLICATE
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13    5.4E+0007  2.000  5000.0  ! MZ 587
     DUPLICATE
!C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    3.0E+0006  2.000  -1520.0  ! MZ 588
     DUPLICATE
!C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    2.7E+0006  2.000  450.0  ! MZ 589
     DUPLICATE
!C10H20Z+R2OH=>H2O+C4H6Z2+R41C6H13    1.5E+0007  2.000  -765.0  ! MZ 590
     DUPLICATE
!C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.4E+0003  2.600  12400.0  ! MZ
591
     DUPLICATE
!C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    6.0E+0011  0.000  17000.0  ! MZ
592
     DUPLICATE
!C10H20Z+R3OOH=>H2O2+C4H6Z2+R41C6H13    2.4E+0012  0.000  15500.0  ! MZ
593
     DUPLICATE
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.0E+0011  0.000  7300.0  ! MZ 594
     DUPLICATE
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    3.0E-0001  4.000  8200.0  ! MZ 595
     DUPLICATE
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13    1.2E+0012  0.000  9600.0  ! MZ 596
     DUPLICATE
!C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.0E+0012  0.000  14550.0  !
MZ 597
     DUPLICATE
!C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    6.0E+0012  0.000  20000.0  !
MZ 598
     DUPLICATE
!C10H20Z+R8CH3OO=>CH3OOH+C4H6Z2+R41C6H13    1.8E+0013  0.000  17500.0  !
MZ 599
     DUPLICATE
!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.5E+0000  3.500  4140.0  ! MZ
600
     DUPLICATE
```

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!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    3.0E+0011  0.000  13500.0  ! MZ
601
     DUPLICATE
!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13    1.2E+0012  0.000  11000.0  ! MZ
602
     DUPLICATE
!C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
603
!C13H26Z+R2OH=>H2O+C4H6Z2+R4CH3+4C2H4Z    3.0E+0006  2.000  -1520.0  ! MZ
604
!C13H26Z+R3OOH=>H2O2+C4H6Z2+R4CH3+4C2H4Z    6.4E+0003  2.600  12400.0  !
MZ 605
!C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0  ! MZ
606
!C13H26Z+R8CH3OO=>CH3OOH+C4H6Z2+R4CH3+4C2H4Z    1.0E+0011  0.000  7300.0
! MZ 607
!C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z    1.5E+0000  3.500  4140.0  !
MZ 608
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    5.4E+0004  2.500  -1900.0  ! MZ 609
     DUPLICATE
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    2.9E+0007  2.000  7700.0  ! MZ 610
     DUPLICATE
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17    7.2E+0007  2.000  5000.0  ! MZ 611
     DUPLICATE
!C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    3.0E+0006  2.000  -1520.0  ! MZ 612
     DUPLICATE
!C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.7E+0006  2.000  450.0  ! MZ 613
     DUPLICATE
!C12H24Z+R2OH=>H2O+C4H6Z2+R30C8H17    2.1E+0007  2.000  -765.0  ! MZ 614
     DUPLICATE
!C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.4E+0003  2.600  12400.0  ! MZ
615
     DUPLICATE
!C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    6.0E+0011  0.000  17000.0  ! MZ
616
     DUPLICATE
!C12H24Z+R3OOH=>H2O2+C4H6Z2+R30C8H17    3.2E+0012  0.000  15500.0  ! MZ
617
     DUPLICATE
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.0E+0011  0.000  7300.0  ! MZ 618
     DUPLICATE
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    3.0E-0001  4.000  8200.0  ! MZ 619
     DUPLICATE
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17    1.6E+0012  0.000  9600.0  ! MZ 620
     DUPLICATE
!C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    1.0E+0012  0.000  14550.0  !
MZ 621
     DUPLICATE
!C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    6.0E+0012  0.000  20000.0  !
MZ 622
     DUPLICATE
!C12H24Z+R8CH3OO=>CH3OOH+C4H6Z2+R30C8H17    2.4E+0013  0.000  17500.0  !
MZ 623
     DUPLICATE
```

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!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.5E+0000  3.500  4140.0  ! MZ
624
     DUPLICATE
!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    3.0E+0011  0.000  13500.0  ! MZ
625
     DUPLICATE
!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17    1.6E+0012  0.000  11000.0  ! MZ
626
     DUPLICATE
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    5.4E+0004  2.500  -1900.0  ! MZ 627
     DUPLICATE
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    2.9E+0007  2.000  7700.0  ! MZ 628
     DUPLICATE
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15    6.3E+0007  2.000  5000.0  ! MZ 629
     DUPLICATE
!C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    3.0E+0006  2.000  -1520.0  ! MZ 630
     DUPLICATE
!C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    2.7E+0006  2.000  450.0  ! MZ 631
     DUPLICATE
!C11H22Z+R2OH=>H2O+C4H6Z2+R26C7H15    1.8E+0007  2.000  -765.0  ! MZ 632
     DUPLICATE
!C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.4E+0003  2.600  12400.0  ! MZ
633
     DUPLICATE
!C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    6.0E+0011  0.000  17000.0  ! MZ
634
     DUPLICATE
!C11H22Z+R3OOH=>H2O2+C4H6Z2+R26C7H15    2.8E+0012  0.000  15500.0  ! MZ
635
     DUPLICATE
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.0E+0011  0.000  7300.0  ! MZ 636
     DUPLICATE
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    3.0E-0001  4.000  8200.0  ! MZ 637
     DUPLICATE
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15    1.4E+0012  0.000  9600.0  ! MZ 638
     DUPLICATE
!C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    1.0E+0012  0.000  14550.0  !
MZ 639
     DUPLICATE
!C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    6.0E+0012  0.000  20000.0  !
MZ 640
     DUPLICATE
!C11H22Z+R8CH3OO=>CH3OOH+C4H6Z2+R26C7H15    2.1E+0013  0.000  17500.0  !
MZ 641
     DUPLICATE
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.5E+0000  3.500  4140.0  ! MZ
642
     DUPLICATE
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    3.0E+0011  0.000  13500.0  ! MZ
643
     DUPLICATE
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15    1.4E+0012  0.000  11000.0  ! MZ
644
     DUPLICATE
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!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z    5.4E+0004  2.500  -1900.0  ! MZ
645
!C14H28Z+R2OH=>H2O+C4H6Z2+R11C2H5+4C2H4Z    3.0E+0006  2.000  -1520.0  !
MZ 646
!C14H28Z+R3OOH=>H2O2+C4H6Z2+R11C2H5+4C2H4Z    6.4E+0003  2.600
12400.0  ! MZ 647
!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000  7300.0  !
MZ 648
!C14H28Z+R8CH3OO=>CH3OOH+C4H6Z2+R11C2H5+4C2H4Z    1.0E+0011  0.000
7300.0  ! MZ 649
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z    1.5E+0000  3.500  4140.0
! MZ 650
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    8.8E+0010  0.700  3250.0  ! MZ 651
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    5.1E+0013  0.000  7850.0  ! MZ 652
     DUPLICATE
C5H10Z+B1O=>R2OH+C4H6Z2+R4CH3    2.6E+0013  0.000  5200.0  ! MZ 653
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    8.8E+0010  0.700  3250.0  ! MZ 654
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    5.1E+0013  0.000  7850.0  ! MZ 655
     DUPLICATE
C7H14Z+B1O=>R2OH+C4H6Z2+R19C3H7    7.8E+0013  0.000  5200.0  ! MZ 656
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    8.8E+0010  0.700  3250.0  ! MZ 657
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.1E+0013  0.000  7850.0  ! MZ 658
     DUPLICATE
C6H12Z+B1O=>R2OH+C4H6Z2+R11C2H5    5.2E+0013  0.000  5200.0  ! MZ 659
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    8.8E+0010  0.700  3250.0  ! MZ 660
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    5.1E+0013  0.000  7850.0  ! MZ 661
     DUPLICATE
C8H16Z+B1O=>R2OH+C4H6Z2+R20C4H9    1.0E+0014  0.000  5200.0  ! MZ 662
     DUPLICATE
!C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    8.8E+0010  0.700  3250.0  ! MZ 663
     DUPLICATE
!C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    5.1E+0013  0.000  7850.0  ! MZ 664
     DUPLICATE
!C9H18Z+B1O=>R2OH+C4H6Z2+R35C5H11    1.3E+0014  0.000  5200.0  ! MZ 665
     DUPLICATE
!C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    8.8E+0010  0.700  3250.0  ! MZ 666
     DUPLICATE
!C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    5.1E+0013  0.000  7850.0  ! MZ 667
     DUPLICATE
!C10H20Z+B1O=>R2OH+C4H6Z2+R41C6H13    1.6E+0014  0.000  5200.0  ! MZ 668
     DUPLICATE
!C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    8.8E+0010  0.700  3250.0  ! MZ 669
     DUPLICATE
!C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    5.1E+0013  0.000  7850.0  ! MZ 670
     DUPLICATE
!C12H24Z+B1O=>R2OH+C4H6Z2+R30C8H17    2.1E+0014  0.000  5200.0  ! MZ 671
     DUPLICATE
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!C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    8.8E+0010  0.700  3250.0  ! MZ 672
     DUPLICATE
!C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    5.1E+0013  0.000  7850.0  ! MZ 673
     DUPLICATE
!C11H22Z+B1O=>R2OH+C4H6Z2+R26C7H15    1.8E+0014  0.000  5200.0  ! MZ 674
     DUPLICATE

! Metathesis with YH
C3H6Y+R1H=>RC3H5Y+H2    1.7E+0005  2.500  2510.0  ! MES 675
C3H6Y+R2OH=>RC3H5Y+H2O    3.0E+0006  2.000  -298.0  ! MES 676
C3H6Y+R3OOH=>RC3H5Y+H2O2    9.6E+0003  2.600  13900.0  ! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4    2.2E+0000  3.500  5670.0  ! MES 678
C3H6Y+R8CH3OO=>RC3H5Y+CH3OOH    2.0E+0012  0.000  17050.0  ! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6    2.2E+0000  3.500  6640.0  ! MES 680
C4H8Y+R1H=>RC4H7Y+H2    5.4E+0004  2.500  -1900.0  ! MES 681
     DUPLICATE
C4H8Y+R1H=>RC4H7Y+H2    2.9E+0007  2.000  7700.0  ! MES 682
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 683
     DUPLICATE
C4H8Y+R2OH=>RC4H7Y+H2O    2.7E+0006  2.000  450.0  ! MES 684
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 685
     DUPLICATE
C4H8Y+R3OOH=>RC4H7Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 686
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    1.0E+0011  0.000  7300.0  ! MES 687
     DUPLICATE
C4H8Y+R4CH3=>RC4H7Y+CH4    3.0E-0001  4.000  8200.0  ! MES 688
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 689
     DUPLICATE
C4H8Y+R8CH3OO=>RC4H7Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 690
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 691
     DUPLICATE
C4H8Y+R11C2H5=>RC4H7Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 692
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    5.4E+0004  2.500  -1900.0  ! MES 693
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.9E+0007  2.000  7700.0  ! MES 694
     DUPLICATE
C7H14Y+R1H=>RC7H13Y+H2    2.7E+0007  2.000  5000.0  ! MES 695
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 696
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    2.7E+0006  2.000  450.0  ! MES 697
     DUPLICATE
C7H14Y+R2OH=>RC7H13Y+H2O    7.8E+0006  2.000  -765.0  ! MES 698
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 699
     DUPLICATE
C7H14Y+R3OOH=>RC7H13Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 700
     DUPLICATE
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C7H14Y+R3OOH=>RC7H13Y+H2O2    1.2E+0012  0.000  15500.0  ! MES 701
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    1.0E+0011  0.000  7300.0  ! MES 702
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    3.0E-0001  4.000  8200.0  ! MES 703
     DUPLICATE
C7H14Y+R4CH3=>RC7H13Y+CH4    6.0E+0011  0.000  9600.0  ! MES 704
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 705
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 706
     DUPLICATE
C7H14Y+R8CH3OO=>RC7H13Y+CH3OOH    9.0E+0012  0.000  17500.0  ! MES 707
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 708
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 709
     DUPLICATE
C7H14Y+R11C2H5=>RC7H13Y+C2H6    6.0E+0011  0.000  11000.0  ! MES 710
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    5.4E+0004  2.500  -1900.0  ! MES 711
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    2.9E+0007  2.000  7700.0  ! MES 712
     DUPLICATE
C8H16Y+R1H=>RC8H15Y+H2    3.6E+0007  2.000  5000.0  ! MES 713
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 714
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    2.7E+0006  2.000  450.0  ! MES 715
     DUPLICATE
C8H16Y+R2OH=>RC8H15Y+H2O    1.0E+0007  2.000  -765.0  ! MES 716
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 717
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 718
     DUPLICATE
C8H16Y+R3OOH=>RC8H15Y+H2O2    1.6E+0012  0.000  15500.0  ! MES 719
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    1.0E+0011  0.000  7300.0  ! MES 720
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    3.0E-0001  4.000  8200.0  ! MES 721
     DUPLICATE
C8H16Y+R4CH3=>RC8H15Y+CH4    8.0E+0011  0.000  9600.0  ! MES 722
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 723
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 724
     DUPLICATE
C8H16Y+R8CH3OO=>RC8H15Y+CH3OOH    1.2E+0013  0.000  17500.0  ! MES 725
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 726
     DUPLICATE
C8H16Y+R11C2H5=>RC8H15Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 727
     DUPLICATE
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C8H16Y+R11C2H5=>RC8H15Y+C2H6    8.0E+0011  0.000  11000.0  ! MES 728
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    5.4E+0004  2.500  -1900.0  ! MES 729
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    2.9E+0007  2.000  7700.0  ! MES 730
     DUPLICATE
C5H10Y+R1H=>RC5H9Y+H2    9.0E+0006  2.000  5000.0  ! MES 731
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    3.0E+0006  2.000  -1520.0  ! MES 732
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.7E+0006  2.000  450.0  ! MES 733
     DUPLICATE
C5H10Y+R2OH=>RC5H9Y+H2O    2.6E+0006  2.000  -765.0  ! MES 734
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.4E+0003  2.600  12400.0  ! MES 735
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    6.0E+0011  0.000  17000.0  ! MES 736
     DUPLICATE
C5H10Y+R3OOH=>RC5H9Y+H2O2    4.0E+0011  0.000  15500.0  ! MES 737
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    1.0E+0011  0.000  7300.0  ! MES 738
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    3.0E-0001  4.000  8200.0  ! MES 739
     DUPLICATE
C5H10Y+R4CH3=>RC5H9Y+CH4    2.0E+0011  0.000  9600.0  ! MES 740
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    1.0E+0012  0.000  14550.0  ! MES 741
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    6.0E+0012  0.000  20000.0  ! MES 742
     DUPLICATE
C5H10Y+R8CH3OO=>RC5H9Y+CH3OOH    3.0E+0012  0.000  17500.0  ! MES 743
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    1.5E+0000  3.500  4140.0  ! MES 744
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    3.0E+0011  0.000  13500.0  ! MES 745
     DUPLICATE
C5H10Y+R11C2H5=>RC5H9Y+C2H6    2.0E+0011  0.000  11000.0  ! MES 746
     DUPLICATE
C3H6Y+B1O=>RC3H5Y+R2OH    1.7E+0011  0.700  5900.0  ! MES 747
C4H8Y+B1O=>RC4H7Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 748
     DUPLICATE
C4H8Y+B1O=>RC4H7Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 749
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 750
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 751
     DUPLICATE
C7H14Y+B1O=>RC7H13Y+R2OH    7.8E+0013  0.000  5200.0  ! MES 752
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 753
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 754
     DUPLICATE
C8H16Y+B1O=>RC8H15Y+R2OH    1.0E+0014  0.000  5200.0  ! MES 755
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     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    8.8E+0010  0.700  3250.0  ! MES 756
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    5.1E+0013  0.000  7850.0  ! MES 757
     DUPLICATE
C5H10Y+B1O=>RC5H9Y+R2OH    2.6E+0013  0.000  5200.0  ! MES 758
     DUPLICATE

! Addition of .Y on YH
RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 759
!RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 760
RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 761
RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 762
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y    6.0E+0009  0.000  11400.0  ! ADY 763
RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 764
!RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 765
!RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 766
RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 767
RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z    6.0E+0009  0.000  11400.0  ! ADY 768
!RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 769
!RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 770
!RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z    6.0E+0009  0.000  11400.0  ! ADY 771
!RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 772
RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 773
!RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 774
!RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z    6.0E+0009  0.000  11400.0  ! ADY 775
!RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z    6.0E+0009  0.000  11400.0  ! ADY 776
!RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 777
!RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z    6.0E+0009  0.000  11400.0  ! ADY 778
RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z    6.0E+0009  0.000  11400.0  ! ADY 779
!RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z    6.0E+0009  0.000  11400.0  ! ADY 780
!RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z    6.0E+0009  0.000  11400.0  ! ADY 781
RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z    6.0E+0009  0.000  11400.0  ! ADY 782
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z    6.0E+0009  0.000  11400.0  ! ADY 783

! Alkohol reactions
C3H7OH+R1H=>H2+R2OH+C3H6Y    2.9E+0007  2.000  7700.0  ! MOL 784
     DUPLICATE
C3H7OH+R1H=>H2+R2OH+C3H6Y    1.8E+0007  2.000  5000.0  ! MOL 785
     DUPLICATE
C3H7OH+R1H=>H2+R11C2H5+HCHO    2.4E+0006  2.000  6525.0  ! MOL 786
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    2.7E+0006  2.000  450.0  ! MOL 787
     DUPLICATE
C3H7OH+R2OH=>H2O+R2OH+C3H6Y    5.2E+0006  2.000  -765.0  ! MOL 788
     DUPLICATE
C3H7OH+R2OH=>H2O+R11C2H5+HCHO    4.0E+0005  2.000  -475.0  ! MOL 789
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    6.0E+0011  0.000  17000.0  ! MOL 790
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R2OH+C3H6Y    8.0E+0011  0.000  15500.0  ! MOL 791
     DUPLICATE
C3H7OH+R3OOH=>H2O2+R11C2H5+HCHO    5.4E+0004  2.000  15025.0  ! MOL 792
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    3.0E-0001  4.000  8200.0  ! MOL 793
     DUPLICATE
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y    4.0E+0011  0.000  9600.0  ! MOL 794
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     DUPLICATE
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO    3.9E+0004  2.000  7525.0  ! MOL 795
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    1.6E+0011  0.000  7300.0  ! MOL 796
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R2OH+C3H6Y    2.9E+0011  0.000  4500.0  ! MOL 797
     DUPLICATE
C3H7OH+R8CH3OO=>CH3OOH+R11C2H5+HCHO    0.0E+0000  0.000  0.0  ! MOL 798
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    3.0E+0011  0.000  13500.0  ! MOL 799
     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y    4.0E+0011  0.000  11000.0  ! MOL 800
     DUPLICATE
C3H7OH+R11C2H5=>C2H6+R11C2H5+HCHO    2.3E+0004  2.000  10525.0  ! MOL 801
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.9E+0007  2.000  7700.0  ! MOL 802
     DUPLICATE
C4H10OL+R1H=>H2+R2OH+C4H8Y    2.7E+0007  2.000  5000.0  ! MOL 803
     DUPLICATE
C4H10OL+R1H=>H2+R19C3H7+HCHO    2.4E+0006  2.000  6525.0  ! MOL 804
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    2.7E+0006  2.000  450.0  ! MOL 805
     DUPLICATE
C4H10OL+R2OH=>H2O+R2OH+C4H8Y    7.8E+0006  2.000  -765.0  ! MOL 806
     DUPLICATE
C4H10OL+R2OH=>H2O+R19C3H7+HCHO    4.0E+0005  2.000  -475.0  ! MOL 807
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    6.0E+0011  0.000  17000.0  ! MOL 808
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R2OH+C4H8Y    1.2E+0012  0.000  15500.0  ! MOL 809
     DUPLICATE
C4H10OL+R3OOH=>H2O2+R19C3H7+HCHO    5.4E+0004  2.000  15025.0  ! MOL 810
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    3.0E-0001  4.000  8200.0  ! MOL 811
     DUPLICATE
C4H10OL+R4CH3=>CH4+R2OH+C4H8Y    6.0E+0011  0.000  9600.0  ! MOL 812
     DUPLICATE
C4H10OL+R4CH3=>CH4+R19C3H7+HCHO    3.9E+0004  2.000  7525.0  ! MOL 813
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    1.6E+0011  0.000  7300.0  ! MOL 814
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R2OH+C4H8Y    4.4E+0011  0.000  4500.0  ! MOL 815
     DUPLICATE
C4H10OL+R8CH3OO=>CH3OOH+R19C3H7+HCHO    0.0E+0000  0.000  0.0  ! MOL 816
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    3.0E+0011  0.000  13500.0  ! MOL 817
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R2OH+C4H8Y    6.0E+0011  0.000  11000.0  ! MOL 818
     DUPLICATE
C4H10OL+R11C2H5=>C2H6+R19C3H7+HCHO    2.3E+0004  2.000  10525.0  ! MOL
819
C5H12OL+R1H=>H2+R2OH+C5H10Z    2.9E+0007  2.000  7700.0  ! MOL 820
     DUPLICATE
C5H12OL+R1H=>H2+R2OH+C5H10Z    3.6E+0007  2.000  5000.0  ! MOL 821
     DUPLICATE
C5H12OL+R1H=>H2+R20C4H9+HCHO    2.4E+0006  2.000  6525.0  ! MOL 822
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    2.7E+0006  2.000  450.0  ! MOL 823
     DUPLICATE
C5H12OL+R2OH=>H2O+R2OH+C5H10Z    1.0E+0007  2.000  -765.0  ! MOL 824
     DUPLICATE
C5H12OL+R2OH=>H2O+R20C4H9+HCHO    4.0E+0005  2.000  -475.0  ! MOL 825
C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    6.0E+0011  0.000  17000.0  ! MOL 826
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     DUPLICATE
C5H12OL+R3OOH=>H2O2+R2OH+C5H10Z    1.6E+0012  0.000  15500.0  ! MOL 827
     DUPLICATE
C5H12OL+R3OOH=>H2O2+R20C4H9+HCHO    5.4E+0004  2.000  15025.0  ! MOL 828
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    3.0E-0001  4.000  8200.0  ! MOL 829
     DUPLICATE
C5H12OL+R4CH3=>CH4+R2OH+C5H10Z    8.0E+0011  0.000  9600.0  ! MOL 830
     DUPLICATE
C5H12OL+R4CH3=>CH4+R20C4H9+HCHO    3.9E+0004  2.000  7525.0  ! MOL 831
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    1.6E+0011  0.000  7300.0  ! MOL
832
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R2OH+C5H10Z    5.8E+0011  0.000  4500.0  ! MOL
833
     DUPLICATE
C5H12OL+R8CH3OO=>CH3OOH+R20C4H9+HCHO    0.0E+0000  0.000  0.0  ! MOL 834
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    3.0E+0011  0.000  13500.0  ! MOL 835
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R2OH+C5H10Z    8.0E+0011  0.000  11000.0  ! MOL 836
     DUPLICATE
C5H12OL+R11C2H5=>C2H6+R20C4H9+HCHO    2.3E+0004  2.000  10525.0  ! MOL
837
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    3.9E+0013  0.000  5200.0  ! MOL 838
     DUPLICATE
C3H7OH+B1O=>R2OH+R2OH+C3H6Y    4.0E+0013  0.000  5200.0  ! MOL 839
     DUPLICATE
C3H7OH+B1O=>R2OH+R11C2H5+HCHO    1.3E+0006  2.000  5025.0  ! MOL 840
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    3.9E+0013  0.000  5200.0  ! MOL 841
     DUPLICATE
C4H10OL+B1O=>R2OH+R2OH+C4H8Y    6.0E+0013  0.000  5200.0  ! MOL 842
     DUPLICATE
C4H10OL+B1O=>R2OH+R19C3H7+HCHO    1.3E+0006  2.000  5025.0  ! MOL 843
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    3.9E+0013  0.000  5200.0  ! MOL 844
     DUPLICATE
C5H12OL+B1O=>R2OH+R2OH+C5H10Z    8.0E+0013  0.000  5200.0  ! MOL 845
     DUPLICATE
C5H12OL+B1O=>R2OH+R20C4H9+HCHO    1.3E+0006  2.000  5025.0  ! MOL 846

! Aldehydes metathesis
C2H5CHO+R1H=>H2+RC3H5O    4.0E+0013  0.000  4200.0  ! ADZ 847
C2H5CHO+R2OH=>H2O+RC3H5O    4.2E+0012  0.000  500.0  ! ADZ 848
C2H5CHO+R3OOH=>H2O2+RC3H5O    1.0E+0012  0.000  10000.0  ! ADZ 849
C2H5CHO+R4CH3=>CH4+RC3H5O    2.0E-0006  5.600  2500.0  ! ADZ 850
C2H5CHO+R11C2H5=>C2H6+RC3H5O    1.3E+0012  0.000  8500.0  ! ADZ 851
C5H10OA+R1H=>H2+RC5H9O    4.0E+0013  0.000  4200.0  ! ADZ 852
C5H10OA+R2OH=>H2O+RC5H9O    4.2E+0012  0.000  500.0  ! ADZ 853
C5H10OA+R3OOH=>H2O2+RC5H9O    1.0E+0012  0.000  10000.0  ! ADZ 854
C5H10OA+R4CH3=>CH4+RC5H9O    2.0E-0006  5.600  2500.0  ! ADZ 855
C5H10OA+R11C2H5=>C2H6+RC5H9O    1.3E+0012  0.000  8500.0  ! ADZ 856
C4H8OA+R1H=>H2+RC4H7O    4.0E+0013  0.000  4200.0  ! ADZ 857
C4H8OA+R2OH=>H2O+RC4H7O    4.2E+0012  0.000  500.0  ! ADZ 858
C4H8OA+R3OOH=>H2O2+RC4H7O    1.0E+0012  0.000  10000.0  ! ADZ 859
C4H8OA+R4CH3=>CH4+RC4H7O    2.0E-0006  5.600  2500.0  ! ADZ 860
C4H8OA+R11C2H5=>C2H6+RC4H7O    1.3E+0012  0.000  8500.0  ! ADZ 861
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C6H12OA+R1H=>H2+RC6H11O    4.0E+0013  0.000  4200.0  ! ADZ 862
C6H12OA+R2OH=>H2O+RC6H11O    4.2E+0012  0.000  500.0  ! ADZ 863
C6H12OA+R3OOH=>H2O2+RC6H11O    1.0E+0012  0.000  10000.0  ! ADZ 864
C6H12OA+R4CH3=>CH4+RC6H11O    2.0E-0006  5.600  2500.0  ! ADZ 865
C6H12OA+R11C2H5=>C2H6+RC6H11O    1.3E+0012  0.000  8500.0  ! ADZ 866
C7H14OA+R1H=>H2+RC7H13O    4.0E+0013  0.000  4200.0  ! ADZ 867
C7H14OA+R2OH=>H2O+RC7H13O    4.2E+0012  0.000  500.0  ! ADZ 868
C7H14OA+R3OOH=>H2O2+RC7H13O    1.0E+0012  0.000  10000.0  ! ADZ 869
C7H14OA+R4CH3=>CH4+RC7H13O    2.0E-0006  5.600  2500.0  ! ADZ 870
C7H14OA+R11C2H5=>C2H6+RC7H13O    1.3E+0012  0.000  8500.0  ! ADZ 871
C8H16OA+R1H=>H2+RC8H15O    4.0E+0013  0.000  4200.0  ! ADZ 872
C8H16OA+R2OH=>H2O+RC8H15O    4.2E+0012  0.000  500.0  ! ADZ 873
C8H16OA+R3OOH=>H2O2+RC8H15O    1.0E+0012  0.000  10000.0  ! ADZ 874
C8H16OA+R4CH3=>CH4+RC8H15O    2.0E-0006  5.600  2500.0  ! ADZ 875
C8H16OA+R11C2H5=>C2H6+RC8H15O    1.3E+0012  0.000  8500.0  ! ADZ 876
!C9H18OA+R1H=>H2+RC9H17O    4.0E+0013  0.000  4200.0  ! ADZ 877
!C9H18OA+R2OH=>H2O+RC9H17O    4.2E+0012  0.000  500.0  ! ADZ 878
!C9H18OA+R3OOH=>H2O2+RC9H17O    1.0E+0012  0.000  10000.0  ! ADZ 879
!C9H18OA+R4CH3=>CH4+RC9H17O    2.0E-0006  5.600  2500.0  ! ADZ 880
!C9H18OA+R11C2H5=>C2H6+RC9H17O    1.3E+0012  0.000  8500.0  ! ADZ 881
!C12H24OA+R1H=>H2+RC12H23O    4.0E+0013  0.000  4200.0  ! ADZ 882
!C12H24OA+R2OH=>H2O+RC12H23O    4.2E+0012  0.000  500.0  ! ADZ 883
!C12H24OA+R3OOH=>H2O2+RC12H23O    1.0E+0012  0.000  10000.0  ! ADZ 884
!C12H24OA+R4CH3=>CH4+RC12H23O    2.0E-0006  5.600  2500.0  ! ADZ 885
!C12H24OA+R11C2H5=>C2H6+RC12H23O    1.3E+0012  0.000  8500.0  ! ADZ 886
!C11H22OA+R1H=>H2+RC11H21O    4.0E+0013  0.000  4200.0  ! ADZ 887
!C11H22OA+R2OH=>H2O+RC11H21O    4.2E+0012  0.000  500.0  ! ADZ 888
!C11H22OA+R3OOH=>H2O2+RC11H21O    1.0E+0012  0.000  10000.0  ! ADZ 889
!C11H22OA+R4CH3=>CH4+RC11H21O    2.0E-0006  5.600  2500.0  ! ADZ 890
!C11H22OA+R11C2H5=>C2H6+RC11H21O    1.3E+0012  0.000  8500.0  ! ADZ 891
!C10H20OA+R1H=>H2+RC10H19O    4.0E+0013  0.000  4200.0  ! ADZ 892
!C10H20OA+R2OH=>H2O+RC10H19O    4.2E+0012  0.000  500.0  ! ADZ 893
!C10H20OA+R3OOH=>H2O2+RC10H19O    1.0E+0012  0.000  10000.0  ! ADZ 894
!C10H20OA+R4CH3=>CH4+RC10H19O    2.0E-0006  5.600  2500.0  ! ADZ 895
!C10H20OA+R11C2H5=>C2H6+RC10H19O    1.3E+0012  0.000  8500.0  ! ADZ 896
!C13H26OA+R1H=>H2+RC13H25O    4.0E+0013  0.000  4200.0  ! ADZ 897
!C13H26OA+R2OH=>H2O+RC13H25O    4.2E+0012  0.000  500.0  ! ADZ 898
!C13H26OA+R3OOH=>H2O2+RC13H25O    1.0E+0012  0.000  10000.0  ! ADZ 899
!C13H26OA+R4CH3=>CH4+RC13H25O    2.0E-0006  5.600  2500.0  ! ADZ 900
!C13H26OA+R11C2H5=>C2H6+RC13H25O    1.3E+0012  0.000  8500.0  ! ADZ 901

C4H6OAY+R1H=>H2+R10C2H3V+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 902
C4H6OAY+R2OH=>H2O+R10C2H3V+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 903
C4H6OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ
904
C4H6OAY+R4CH3=>CH4+R10C2H3V+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 905
C4H6OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
906
C5H8OAY+R1H=>H2+RC3H5Y+CH2COZ    4.0E+0013  0.000  4200.0  ! ADZ 907
C5H8OAY+R2OH=>H2O+RC3H5Y+CH2COZ    4.0E+0012  0.000  500.0  ! ADZ 908
C5H8OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ    1.0E+0012  0.000  10000.0  ! ADZ 909
C5H8OAY+R4CH3=>CH4+RC3H5Y+CH2COZ    2.0E-0006  0.000  2500.0  ! ADZ 910
C5H8OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ    1.3E+0012  0.000  8500.0  ! ADZ
911
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!C8H14OAY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 912
!C8H14OAY+R2OH=>H2O+R10C2H3V+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 913
!C8H14OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+2C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 914
!C8H14OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z    2.0E-0006  0.000
2500.0  ! ADZ 915
!C8H14OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z    1.3E+0012  0.000
8500.0  ! ADZ 916
!C9H16OAY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0013  0.000  4200.0  ! ADZ
917
!C9H16OAY+R2OH=>H2O+RC3H5Y+CH2COZ+2C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 918
!C9H16OAY+R3OOH=>H2O2+RC3H5Y+CH2COZ+2C2H4Z    1.0E+0012  0.000
10000.0  ! ADZ 919
!C9H16OAY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 920
!C9H16OAY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 921
!C6H10OAY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z    4.0E+0013  0.000  4200.0  !
ADZ 922
!C6H10OAY+R2OH=>H2O+R10C2H3V+CH2COZ+C2H4Z    4.0E+0012  0.000  500.0  !
ADZ 923
!C6H10OAY+R3OOH=>H2O2+R10C2H3V+CH2COZ+C2H4Z    1.0E+0012  0.000  10000.0
! ADZ 924
!C6H10OAY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z    2.0E-0006  0.000  2500.0  !
ADZ 925
!C6H10OAY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z    1.3E+0012  0.000  8500.0
! ADZ 926

! Keto radicals decomposition
RC3H5O=>B2CO+R11C2H5    1.8E+0014  0.000  15600.0  ! COR 927
RC5H9O=>B2CO+R20C4H9    1.8E+0014  0.000  15600.0  ! COR 928
RC4H7O=>B2CO+R19C3H7    1.8E+0014  0.000  15600.0  ! COR 929
RC6H11O=>B2CO+R35C5H11    1.8E+0014  0.000  15600.0  ! COR 930
RC7H13O=>B2CO+R41C6H13    1.8E+0014  0.000  15600.0  ! COR 931
RC8H15O=>B2CO+R26C7H15    1.8E+0014  0.000  15600.0  ! COR 932
!RC9H17O=>B2CO+R30C8H17    1.8E+0014  0.000  15600.0  ! COR 933
!RC12H23O=>B2CO+R4CH3+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 934
!RC11H21O=>B2CO+R11C2H5+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 935
!RC10H19O=>B2CO+R4CH3+4C2H4Z    1.8E+0014  0.000  15600.0  ! COR 936
!RC13H25O=>B2CO+R11C2H5+5C2H4Z    1.8E+0014  0.000  15600.0  ! COR 937


! keto radicals addition to O2
RC3H5O+O2=>RC3H5O3    3.0E+0019  -2.500  0.0  ! COR 938
RC5H9O+O2=>RC5H9O3    3.0E+0019  -2.500  0.0  ! COR 939
RC4H7O+O2=>RC4H7O3    3.0E+0019  -2.500  0.0  ! COR 940
RC6H11O+O2=>RC6H11O3    3.0E+0019  -2.500  0.0  ! COR 941
RC7H13O+O2=>RC7H13O3    3.0E+0019  -2.500  0.0  ! COR 942
RC8H15O+O2=>RC8H15O3    3.0E+0019  -2.500  0.0  ! COR 943
!RC9H17O+O2=>RC9H17O3    3.0E+0019  -2.500  0.0  ! COR 944
!RC12H23O+O2=>RC12H23O3    3.0E+0019  -2.500  0.0  ! COR 945
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!RC11H21O+O2=>RC11H21O3    3.0E+0019  -2.500  0.0  ! COR 946
!RC10H19O+O2=>RC10H19O3    3.0E+0019  -2.500  0.0  ! COR 947
!RC13H25O+O2=>RC13H25O3    3.0E+0019  -2.500  0.0  ! COR 948

! Peracide radical decomposition
RC3H5O3=>C2H4Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 949
RC5H9O3=>C4H8Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 950
RC4H7O3=>C3H6Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 951
RC6H11O3=>C5H10Y+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 952
RC7H13O3=>C6H12Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 953
RC8H15O3=>C7H14Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 954
!RC9H17O3=>C8H16Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 955
!RC12H23O3=>C11H22Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 956
!RC11H21O3=>C10H20Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 957
!RC10H19O3=>C9H18Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 958
!RC13H25O3=>C12H24Z+R2OH+CO2    4.5E+0011  0.000  25000.0  ! PER 959

! Ketones reactions
!C2H6CO+R1H=>H2+CH2COZ+R4CH3    5.7E+0007  2.000  7700.0  ! MK 960
!C2H6CO+R2OH=>H2O+CH2COZ+R4CH3    5.4E+0006  2.000  450.0  ! MK 961
!C2H6CO+R3OOH=>H2O2+CH2COZ+R4CH3    1.2E+0012  0.000  17000.0  ! MK 962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3    6.0E-0001  4.000  8200.0  ! MK 963
!C2H6CO+R8CH3OO=>CH3OOH+CH2COZ+R4CH3    1.2E+0013  0.000  20000.0  ! MK
964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3    6.0E+0011  0.000  13500.0  ! MK 965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    5.7E+0007  2.000  7700.0  ! MK 966
     DUPLICATE
C3H8CO+R1H=>H2+CH2COZ+R11C2H5    9.0E+0006  2.000  5000.0  ! MK 967
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    5.4E+0006  2.000  450.0  ! MK 968
     DUPLICATE
C3H8CO+R2OH=>H2O+CH2COZ+R11C2H5    2.6E+0006  2.000  -765.0  ! MK 969
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    1.2E+0012  0.000  17000.0  ! MK 970
     DUPLICATE
C3H8CO+R3OOH=>H2O2+CH2COZ+R11C2H5    4.0E+0011  0.000  15500.0  ! MK 971
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    6.0E-0001  4.000  8200.0  ! MK 972
     DUPLICATE
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5    2.0E+0011  0.000  9600.0  ! MK 973
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    1.2E+0013  0.000  20000.0  ! MK
974
     DUPLICATE
C3H8CO+R8CH3OO=>CH3OOH+CH2COZ+R11C2H5    3.0E+0012  0.000  17500.0  ! MK
975
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    6.0E+0011  0.000  13500.0  ! MK
976
     DUPLICATE
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5    2.0E+0011  0.000  11000.0  ! MK
977
     DUPLICATE
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! Unsaturated ester reactions
! Esters metatesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis
! Addition on unsaturated esters

! Carboxylic acid reactions
! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alkohol ene to dienes
C3H6OLY+R1H=>H2+HCHO+R10C2H3V    5.4E+0004  2.500  -1900.0  ! ROH 978
C3H6OLY+R2OH=>H2O+HCHO+R10C2H3V    3.0E+0006  2.000  -1520.0  ! ROH 979
C3H6OLY+R3OOH=>H2O2+HCHO+R10C2H3V    6.4E+0003  2.600  12400.0  ! ROH 980
C3H6OLY+R4CH3=>CH4+HCHO+R10C2H3V    1.0E+0011  0.000  7300.0  ! ROH 981
C3H6OLY+R8CH3OO=>CH3OOH+HCHO+R10C2H3V    1.0E+0012  0.000  14550.0  ! ROH
982
C3H6OLY+R11C2H5=>C2H6+HCHO+R10C2H3V    1.5E+0000  3.500  4140.0  ! ROH
983
C4H8OLY+R1H=>H2+HCHO+RC3H5Y    5.4E+0004  2.500  -1900.0  ! ROH 984
C4H8OLY+R2OH=>H2O+HCHO+RC3H5Y    3.0E+0006  2.000  -1520.0  ! ROH 985
C4H8OLY+R3OOH=>H2O2+HCHO+RC3H5Y    6.4E+0003  2.600  12400.0  ! ROH 986
C4H8OLY+R4CH3=>CH4+HCHO+RC3H5Y    1.0E+0011  0.000  7300.0  ! ROH 987
C4H8OLY+R8CH3OO=>CH3OOH+HCHO+RC3H5Y    1.0E+0012  0.000  14550.0  ! ROH
988
C4H8OLY+R11C2H5=>C2H6+HCHO+RC3H5Y    1.5E+0000  3.500  4140.0  ! ROH 989
C5H10OLY+R1H=>H2+HCHO+RC4H7Y    5.4E+0004  2.500  -1900.0  ! ROH 990
C5H10OLY+R2OH=>H2O+HCHO+RC4H7Y    3.0E+0006  2.000  -1520.0  ! ROH 991
C5H10OLY+R3OOH=>H2O2+HCHO+RC4H7Y    6.4E+0003  2.600  12400.0  ! ROH 992
C5H10OLY+R4CH3=>CH4+HCHO+RC4H7Y    1.0E+0011  0.000  7300.0  ! ROH 993
C5H10OLY+R8CH3OO=>CH3OOH+HCHO+RC4H7Y    1.0E+0012  0.000  14550.0  ! ROH
994
C5H10OLY+R11C2H5=>C2H6+HCHO+RC4H7Y    1.5E+0000  3.500  4140.0  ! ROH 995
C7H14OLY+R1H=>H2+HCHO+RC6H11Y    5.4E+0004  2.500  -1900.0  ! ROH 996
C7H14OLY+R2OH=>H2O+HCHO+RC6H11Y    3.0E+0006  2.000  -1520.0  ! ROH 997
C7H14OLY+R3OOH=>H2O2+HCHO+RC6H11Y    6.4E+0003  2.600  12400.0  ! ROH 998
C7H14OLY+R4CH3=>CH4+HCHO+RC6H11Y    1.0E+0011  0.000  7300.0  ! ROH 999
C7H14OLY+R8CH3OO=>CH3OOH+HCHO+RC6H11Y    1.0E+0012  0.000  14550.0  ! ROH
1000
C7H14OLY+R11C2H5=>C2H6+HCHO+RC6H11Y    1.5E+0000  3.500  4140.0  ! ROH
1001
C8H16OLY+R1H=>H2+HCHO+RC7H13Y    5.4E+0004  2.500  -1900.0  ! ROH 1002
C8H16OLY+R2OH=>H2O+HCHO+RC7H13Y    3.0E+0006  2.000  -1520.0  ! ROH 1003
C8H16OLY+R3OOH=>H2O2+HCHO+RC7H13Y    6.4E+0003  2.600  12400.0  ! ROH
1004
C8H16OLY+R4CH3=>CH4+HCHO+RC7H13Y    1.0E+0011  0.000  7300.0  ! ROH 1005
C8H16OLY+R8CH3OO=>CH3OOH+HCHO+RC7H13Y    1.0E+0012  0.000  14550.0  ! ROH
1006
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C8H16OLY+R11C2H5=>C2H6+HCHO+RC7H13Y    1.5E+0000  3.500  4140.0  ! ROH
1007
!C9H18OLY+R1H=>H2+HCHO+RC8H15Y    5.4E+0004  2.500  -1900.0  ! ROH 1008
!C9H18OLY+R2OH=>H2O+HCHO+RC8H15Y    3.0E+0006  2.000  -1520.0  ! ROH 1009
!C9H18OLY+R3OOH=>H2O2+HCHO+RC8H15Y    6.4E+0003  2.600  12400.0  ! ROH
1010
!C9H18OLY+R4CH3=>CH4+HCHO+RC8H15Y    1.0E+0011  0.000  7300.0  ! ROH 1011
!C9H18OLY+R8CH3OO=>CH3OOH+HCHO+RC8H15Y    1.0E+0012  0.000  14550.0  !
ROH 1012
!C9H18OLY+R11C2H5=>C2H6+HCHO+RC8H15Y    1.5E+0000  3.500  4140.0  ! ROH
1013
C6H12OLY+R1H=>H2+HCHO+RC5H9Y    5.4E+0004  2.500  -1900.0  ! ROH 1014
C6H12OLY+R2OH=>H2O+HCHO+RC5H9Y    3.0E+0006  2.000  -1520.0  ! ROH 1015
C6H12OLY+R3OOH=>H2O2+HCHO+RC5H9Y    6.4E+0003  2.600  12400.0  ! ROH 1016
C6H12OLY+R4CH3=>CH4+HCHO+RC5H9Y    1.0E+0011  0.000  7300.0  ! ROH 1017
C6H12OLY+R8CH3OO=>CH3OOH+HCHO+RC5H9Y    1.0E+0012  0.000  14550.0  ! ROH
1018
C6H12OLY+R11C2H5=>C2H6+HCHO+RC5H9Y    1.5E+0000  3.500  4140.0  ! ROH
1019

! Additions on dienes
C4H6Z2+R2OH=>RC3H5Y+HCHO    1.4E+0012  0.000  -1040.0  ! AD 1020!!!!!!ds
мйса toluиne
!
!C4H6Z2+R2OH=>RC3H5Y+HCHO    3.0E+0012  0.000  -1040.0  !
!
C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V    1.0E+0005  2.500  -1900.0  ! AD 1021
C6H10Y2+R2OH=>H2O+C4H6Z2+R10C2H3V    6.0E+0006  2.000  -1520.0  ! AD 1022
C6H10Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V    1.2E+0004  2.600  12400.0  ! AD
1023
C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD 1024
C6H10Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V    2.0E+0011  0.000  7300.0  ! AD
1025
C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V    3.0E+0000  3.500  4140.0  ! AD
1026
C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y    1.0E+0005  2.500  -1900.0  ! AD 1027
C7H12Y2+R2OH=>H2O+C4H6Z2+RC3H5Y    6.0E+0006  2.000  -1520.0  ! AD 1028
C7H12Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y    1.2E+0004  2.600  12400.0  ! AD 1029
C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD 1030
C7H12Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y    2.0E+0011  0.000  7300.0  ! AD
1031
C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y    3.0E+0000  3.500  4140.0  ! AD
1032
!C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1033
!C10H18Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+2C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1034
!C10H18Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z    1.2E+0004  2.600  12400.0
! AD 1035
!C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1036
!C10H18Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1037
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!C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1038
!C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1039
!C11H20Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+2C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1040
!C11H20Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1041
!C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1042
!C11H20Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+2C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1043
!C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z    3.0E+0000  3.500  4140.0
! AD 1044
!C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1045
!C8H14Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1046
!C8H14Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1047
!C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1048
!C8H14Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1049
!C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z    3.0E+0000  3.500  4140.0
! AD 1050
!C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1051
!C12H22Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+3C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1052
!C12H22Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+3C2H4Z    1.2E+0004  2.600  12400.0
! AD 1053
!C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1054
!C12H22Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1055
!C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1056
!C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1057
!C9H16Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+C2H4Z    6.0E+0006  2.000  -1520.0  ! AD
1058
!C9H16Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+C2H4Z    1.2E+0004  2.600  12400.0  !
AD 1059
!C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0  ! AD
1060
!C9H16Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+C2H4Z    2.0E+0011  0.000  7300.0
! AD 1061
!C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z    3.0E+0000  3.500  4140.0  !
AD 1062
!C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1063
!C14H26Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+4C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1064
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!C14H26Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+4C2H4Z    1.2E+0004  2.600  12400.0
! AD 1065
!C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1066
!C14H26Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1067
!C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1068
!C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1069
!C15H28Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+4C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1070
!C15H28Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+4C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1071
!C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1072
!C15H28Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+4C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1073
!C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z    3.0E+0000  3.500  4140.0
! AD 1074
!C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z    1.0E+0005  2.500  -1900.0  !
AD 1075
!C16H30Y2+R2OH=>H2O+C4H6Z2+R10C2H3V+5C2H4Z    6.0E+0006  2.000
-1520.0  ! AD 1076
!C16H30Y2+R3OOH=>H2O2+C4H6Z2+R10C2H3V+5C2H4Z    1.2E+0004  2.600  12400.0
! AD 1077
!C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1078
!C16H30Y2+R8CH3OO=>CH3OOH+C4H6Z2+R10C2H3V+5C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1079
!C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z    3.0E+0000  3.500
4140.0  ! AD 1080
!C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z    1.0E+0005  2.500  -1900.0  ! AD
1081
!C13H24Y2+R2OH=>H2O+C4H6Z2+RC3H5Y+3C2H4Z    6.0E+0006  2.000  -1520.0  !
AD 1082
!C13H24Y2+R3OOH=>H2O2+C4H6Z2+RC3H5Y+3C2H4Z    1.2E+0004  2.600
12400.0  ! AD 1083
!C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000  7300.0  !
AD 1084
!C13H24Y2+R8CH3OO=>CH3OOH+C4H6Z2+RC3H5Y+3C2H4Z    2.0E+0011  0.000
7300.0  ! AD 1085
!C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z    3.0E+0000  3.500  4140.0
! AD 1086

! Diels Alder

! .Y termination
RC3H5Y+R1H=>C3H6Y    1.0E+0014  0.000  0.0  ! TER
1087 !!!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC3H5Y+R2OH=>C3H6OLY    1.0E+0013  0.000  0.0  ! TER 1088
RC3H5Y+R3OOH=>C3H6O2PY    5.0E+0012  0.000  0.0  ! TER 1089
RC3H5Y+R4CH3=>C4H8Y    1.0E+0013  0.000  0.0  ! TER 1090
RC3H5Y+R5CHO=>C4H6OAY    1.0E+0013  0.000  0.0  ! TER 1091
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RC3H5Y+R6CH2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1092
RC3H5Y+R8CH3OO=>HCHO+R7CH3O+R10C2H3V    1.0E+0013  0.000  0.0  ! TER 1093
RC3H5Y+R11C2H5=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1094
RC4H7Y+R1H=>C4H8Y    1.0E+0014  0.000  0.0  ! TER
1095!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC4H7Y+R2OH=>C4H8OLY    1.0E+0013  0.000  0.0  ! TER 1096
RC4H7Y+R3OOH=>C4H8O2PY    5.0E+0012  0.000  0.0  ! TER 1097
RC4H7Y+R4CH3=>C5H10Y    1.0E+0013  0.000  0.0  ! TER 1098
RC4H7Y+R5CHO=>C5H8OAY    1.0E+0013  0.000  0.0  ! TER 1099
RC4H7Y+R6CH2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1100
RC4H7Y+R8CH3OO=>HCHO+R7CH3O+RC3H5Y    1.0E+0013  0.000  0.0  ! TER 1101
RC4H7Y+R11C2H5=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1102
RC7H13Y+R1H=>C7H14Y    1.0E+0014  0.000  0.0  ! TER
1103!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC7H13Y+R2OH=>C7H14OLY    1.0E+0013  0.000  0.0  ! TER 1104
RC7H13Y+R3OOH=>C7H14O2PY    5.0E+0012  0.000  0.0  ! TER 1105
RC7H13Y+R4CH3=>C8H16Y    1.0E+0013  0.000  0.0  ! TER 1106
RC7H13Y+R5CHO=>C8H14OAY    1.0E+0013  0.000  0.0  ! TER 1107
RC7H13Y+R6CH2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1108
RC7H13Y+R8CH3OO=>HCHO+R7CH3O+RC6H11Y    1.0E+0013  0.000  0.0  ! TER 1109
!RC7H13Y+R11C2H5=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1110
RC8H15Y+R1H=>C8H16Y    1.0E+0014  0.000  0.0  ! TER
1111!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC8H15Y+R2OH=>C8H16OLY    1.0E+0013  0.000  0.0  ! TER 1112
RC8H15Y+R3OOH=>C8H16O2PY    5.0E+0012  0.000  0.0  ! TER 1113
!RC8H15Y+R4CH3=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1114
!RC8H15Y+R5CHO=>C9H16OAY    1.0E+0013  0.000  0.0  ! TER 1115
!RC8H15Y+R6CH2OH=>C9H18OLY    1.0E+0013  0.000  0.0  ! TER 1116
RC8H15Y+R8CH3OO=>HCHO+R7CH3O+RC7H13Y    1.0E+0013  0.000  0.0  ! TER 1117
!RC8H15Y+R11C2H5=>C10H20Z    1.0E+0013  0.000  0.0  ! TER 1118
RC5H9Y+R1H=>C5H10Y    1.0E+0014  0.000  0.0  ! TER
1119!!!!!!!!!!!!!!!!!!!!!!multiplій x10
RC5H9Y+R2OH=>C5H10OLY    1.0E+0013  0.000  0.0  ! TER 1120
RC5H9Y+R3OOH=>C5H10O2PY    5.0E+0012  0.000  0.0  ! TER 1121
RC5H9Y+R4CH3=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1122
RC5H9Y+R5CHO=>C6H10OAY    1.0E+0013  0.000  0.0  ! TER 1123
RC5H9Y+R6CH2OH=>C6H12OLY    1.0E+0013  0.000  0.0  ! TER 1124
RC5H9Y+R8CH3OO=>HCHO+R7CH3O+RC4H7Y    1.0E+0013  0.000  0.0  ! TER 1125
RC5H9Y+R11C2H5=>C7H14Y    1.0E+0013  0.000  0.0  ! TER 1126
RC3H5Y+RC3H5Y=>C6H10Y2    1.0E+0013  0.000  0.0  ! TER 1127
RC3H5Y+RC4H7Y=>C7H12Y2    1.0E+0013  0.000  0.0  ! TER 1128
RC3H5Y+RC7H13Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1129
RC3H5Y+RC8H15Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1130
RC3H5Y+RC5H9Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1131
RC4H7Y+RC4H7Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1132
RC4H7Y+RC7H13Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1133
!RC4H7Y+RC8H15Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1134
RC4H7Y+RC5H9Y=>C9H16Y2    1.0E+0013  0.000  0.0  ! TER 1135
!RC7H13Y+RC7H13Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1136
!RC7H13Y+RC8H15Y=>C15H28Y2    1.0E+0013  0.000  0.0  ! TER 1137
!RC7H13Y+RC5H9Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1138
!RC8H15Y+RC8H15Y=>C16H30Y2    1.0E+0013  0.000  0.0  ! TER 1139
!RC8H15Y+RC5H9Y=>C13H24Y2    1.0E+0013  0.000  0.0  ! TER 1140
!RC8H15Y+RC6H11Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1141
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RC5H9Y+RC5H9Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1142
RC5H9Y+RC6H11Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1143

!
*********************************************************************
**!
!especes excitees!
R1H+B1O+M=OHE+M                    6.0E14      0.0      6.94E3     !
<HALL05>!
B4CH+O2=B2CO+OHE                   4.0E13      0.0      0.0        !
<HALL05>!
OHE+AR=R2OH+AR                     5.2E10      0.5      0.0        !
<HALL05>!
OHE+H2O=R2OH+H2O                   8.6E12      0.5      0.0        !
<HALL05>!
OHE+H2=R2OH+H2                     1.5E12      0.5      0.0        !
<HALL05>!
OHE+R1H=R2OH+R1H                   1.5E12      0.5      0.0        !
<HALL05>!
OHE+O2=R2OH+O2                     1.5E12      0.5      0.0        !
<HALL05>!
OHE+B1O=R2OH+B1O                   1.5E12      0.5      0.0        !
<HALL05>!
OHE+R2OH=R2OH+R2OH                 1.5E12      0.5      0.0        !
<HALL05>!
OHE=>R2OH                             1.4E6       0.0      0.0        !
<HALL05>!
OHE+CO2=R2OH+CO2                   2.75E12     0.5     -968.      !
<HALL05>!
OHE+B2CO=R2OH+B2CO                 3.23E12     0.5     -787.      !
<HALL05>!
OHE+CH4=R2OH+CH4                   3.36E12     0.5     -635.      !
<HALL05>!
R9C2H+B1O=B2CO+CHE                 6.2E12      0.0      0.0        !
<HALL05>!
R9C2H+O2=CO2+CHE                   2.17E10     0.0      0.0        !
<HALL05>!
CHE+AR=B4CH+AR                     4.0E10      0.5      0.0        !
<HALL05>!
CHE+O2=B4CH+O2                     2.48E6      2.14     0.0        !
<HALL05>!
CHE+H2O=B4CH+H2O                   5.3E13      0.0      0.0        !
<HALL05>!
CHE+H2=B4CH+H2                     1.47E14     0.0      1360.      !
<HALL05>!
CHE+CO2=B4CH+CO2                   2.41E-1     4.3     -1694.          !
<HALL05>!
CHE+B2CO=B4CH+B2CO                 2.44E12     0.5      0.0       !
<HALL05>!
CHE+CH4=B4CH+CH4                   1.73E13     0.0      167.      !
<HALL05>!
CHE=>B4CH                             1.86E6      0.0      0.0        !
<HALL05>!
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!*******************************************!
!    REACTIONS DE LA MATRICE O(0)C(y)H(z)   !
!*******************************************!

!****** REACTIONS DE H2******!
R1H+R1H+M=H2+M               1.87E18     -1.00     0.00
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/
AR/0.35/
!      N2/0.4/ HE/0.35/

!****** REACTIONS DE B4CH ******!
B4CH+R1H=B3C+H2             7.8E13       0.       0.       !(2,-
2)<PEETERS97>!

!****** REACTIONS DE B6CH2 ******!
B6CH2+M=B5CH2+M              1.51E13      0.0      0.0
       O2/.4/ B2CO/.75/ CO2/1.5/ H2O/6.5/ CH4/.48/  C2H4Z/1.6/
      AR/.24/
B6CH2+R1H=B4CH+H2            3.0E13       0.       0.           !(4,-
4)<TSAnG86>!

!****** REACTIONS DE B5CH2 ******!
B5CH2+R1H=B4CH+H2            6.0E12       0.      -1.8E3        !(5,-
5)<BAULCH94>!
B5CH2+B3C=R9C2H+R1H         5.0E13       0.       0.           !(6,-
6)<RAnZI94>!
B5CH2+B5CH2=>C2H2+R1H+R1H    1.2E14       0.       0.8E3        !
(7)<BAULCH94>!

!****** REACTIONS DE R4CH3 ******!
R4CH3+M=B5CH2+R1H+M              2.91E16     0.0     90.7E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R4CH3+R1H=B6CH2+H2            6.0E13      0.        15.0E3           !
(9,-9)<BAULCH94>!
R4CH3+B4CH=R10C2H3V+R1H       3.0E13      0.         0.          !(10,-
10)<DAGAUT91>
R4CH3+B6CH2=C2H4Z+R1H         1.8E13      0.         0.          !(11,-
11)<TSAnG86>!
R4CH3+B5CH2=C2H4Z+R1H         4.2E13      0.         0.          !(12,-
12)<BAULCH94>!
R4CH3+B3C=C2H2+R1H           5.0E13      0.         0.          !(13,-
13)<RAnZI94>!
R4CH3+R4CH3(+M)=>C2H6(+M)     3.61E13     0.         0.          !
(14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.63E41  -7.0   2.76E3 /
      TROE /  0.62  73  1180 /
C2H6(+M)=>R4CH3+R4CH3(+M)     1.8E21      -1.24    90.9E3       !(-
14)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
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      LOW / 1.89E49   -8.24   93.7E3/
      TROE /  0.62  73  1180 /
R4CH3+R4CH3=R11C2H5+R1H        3.0E13      0.      13.5E3        !(15,-
15)<BAULCH94>!
R4CH3+R4CH3=C2H4Z+H2           2.1E14      0.      19.3E3        !(16,-
16)<FRAnK86nIST>!

!****** REACTIONS DE CH4 ******!
R1H+R4CH3(+M)=>CH4(+M)         1.67E14     0.      0.            !
(17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW /  1.408E24  -1.8   0.0 /
      TROE / 0.37 3315 61 /
CH4(+M)=>R4CH3+R1H(+M)         2.4E16      0.    105.0E3         !(-
17)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/
!     N2/0.4/ HE/0.35/
      LOW / 1.29E18    0.00  90.9E3 /
      TROE / 0  1350  1  7830 /
CH4(+CH4)=>R4CH3+R1H(+CH4)     2.4E16      0.    105.0E3         !(-
17')<BAULCH94>!
      LOW / 8.43E17    0.00  90.9E3 /
      TROE / 0.69  90  2210 /
CH4+R1H=R4CH3+H2               1.3E04      3.      8.0E3         !(18,-
18)<BAULCH94>!
CH4+B4CH=C2H4Z+R1H             3.0E13      0.     -0.4E3         !(19,-
19)<DAGAUT91BAULCH94>!
CH4+B6CH2=R4CH3+R4CH3          4.2E13      0.      0.            !(20,-
20)<TSAnG86>!

!****** REACTIONS DE R9C2H ******!
R9C2H+B6CH2=C2H2+B4CH          1.8E13      0.         0.         !(21,-
21)<TSAnG86>!
R9C2H+B5CH2=C2H2+B4CH          1.8E13      0.         0.         !(22,-
22)<TSAnG86>!
R9C2H+CH4=C2H2+R4CH3           1.2E12      0.         0.         !(23,-
23)<BAULCH94>!

!****** REACTIONS DE C2H2 ******!
C2H2+M=R9C2H+R1H+M             1.14E17     0.    107.0E3         !(24,-
24)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H2+R1H=R9C2H+H2              6.6E13      0.     27.7E3         !(25,-
25)<BAULCH94>!

!****** REACTIONS DE R10C2H3V ******!
R10C2H3V(+M)=C2H2+R1H(+M)      2.0E14      0.     39.8E3         !(26,-
26)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 1.19E42  -7.50  45.55E3 /
      TROE    /0.35   1.0       1.E8/
```

```
R10C2H3V+R1H=C2H2+H2          1.2E13      0.          0.          !(27,-
27)<BAULCH94>!
R10C2H3V+B6CH2=C2H2+R4CH3     1.8E13      0.          0.          !(28,-
28)<TSAnG86>!
R10C2H3V+B5CH2=C2H2+R4CH3     1.8E13      0.          0.          !(29,-
29)<TSAnG86>!
R10C2H3V+R4CH3=CH4+C2H2       3.9E11      0.          0.          !(30,-
30)<TSAnG86>!
R10C2H3V+R9C2H=2C2H2          9.6E11      0.          0.          !(31,-
31)<TSAnG86>!
R10C2H3V+R10C2H3V=C2H4Z+C2H2  9.6E11      0.          0.          !(32,-
32)<TSAnG86>!

!****** REACTIONS DE C2H4Z ******!
C2H4Z+M=C2H2+H2+M             9.97E16     0.     71.6E3          !(33,-
33)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
C2H4Z+M=R10C2H3V+R1H+M        7.40E17     0.     96.7E3          !(34,-
34)<BAULCH94>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!C2H4Z+R1H=R10C2H3V+H2        5.4E14      0.     14.8E3          !(35,-
35)<BAULCH94>!
C2H4Z+R1H=R10C2H3V+H2         5.0E7       1.93   13.0E3          !(35,-
35)SLAGLE96!
!C2H4Z+R4CH3=CH4+R10C2H3V     4.1E12      0.     11.1E3          !(36,-
36)<BAULCH94>!
C2H4Z+R4CH3=CH4+R10C2H3V      6.3E11      0.     16.0E3          !(36,-
36)BACK89!

!****** REACTIONS DE R11C2H5 ******!
!C2H4Z+R1H(+M)=>R11C2H5(+M)    3.97E09    1.28     1.3E3
!      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
!      LOW / 1.35E19   0.00   0.76E3 /
!      TROE / 0.76  40  1025/
R11C2H5(+M)=C2H4Z+R1H(+M)      8.2E13      0.    40.0E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
      LOW / 3.40E17   0.00   33.4E3 /
      TROE / 0.75  97  1379/
R11C2H5+R1H=C2H4Z+H2           1.8E12      0.          0.          !(38,-
38)<TSAnG86>!
R11C2H5+R1H=C2H6               3.6E13      0.          0.          !(39,-
39><TSAnG86>!
R11C2H5+B6CH2=C2H4Z+R4CH3      9.0E12      0.          0.          !(40,-
40)<TSAnG86>!
R11C2H5+B5CH2=C2H4Z+R4CH3      1.8E13      0.          0.          !(41,-
41)<TSAnG86>!
R11C2H5+R4CH3=C2H4Z+CH4        1.1E12      0.          0.          !(42,-
42)<BAULCH94>!
R11C2H5+R9C2H=C2H2+C2H4Z       1.8E12      0           0.          !(43,-
43)<TSAnG86>!
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R11C2H5+R10C2H3V=2C2H4Z        4.8E11      0.          0.         !(44,-
44)<TSAnG86>!
R11C2H5+R10C2H3V=C2H2+C2H6     4.8E11      0.          0.         !(45,-
45)<TSAnG86>!
R11C2H5+R11C2H5=C2H4Z+C2H6     1.4E12      0.          0.         !(46,-
46)<BAULCH94>!

!****** REACTIONS DE C2H6 ******!
C2H6+M=C2H4Z+H2+M              2.3E17      0.      67.4E3         !(47,-
47)<SCHULTZ85nIST>!
C2H6+R1H=R11C2H5+H2            1.4E9       1.5      7.4E3         !(48,-
48)<BAULCH94>!
C2H6+B6CH2=R4CH3+R11C2H5       1.1E14      0.          0.         !(49,-
49)<TSAnG86>!
C2H6+R4CH3=R11C2H5+CH4         1.5E-7      6.0      5.8E3         !(50,-
50)<BAULCH94>!
C2H6+R9C2H=C2H2+R11C2H5        3.6E12      0.          0.         !(51,-
51)<TSAnG86>!
C2H6+R10C2H3V=R11C2H5+C2H4Z    6.0E2       3.3     10.5E3         !(52,-
52)<TSAnG86>!


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!*****************************************************!
!          REACTIONS DE LA MATRICE O(x)C(y)H(z)  x>0      !
!*****************************************************!

!****** REACTIONS DE B1O ******!
B1O+H2=R2OH+R1H                5.1E4       2.67     6.2E3         !(53,-
53)<BAULCH94>!
B1O+B4CH=B2CO+R1H              3.9E13      0.          0.         !(54,-
54)<BAULCH94>!
B1O+B4CH=B3C+R2OH             1.5E13      0.      4.7E3          !(55,-
55)<MUR86nIS>!
B1O+B6CH2=>B2CO+2R1H           1.5E13      0.          0.         !(56)
<TSAnG86>!
B1O+B6CH2=B2CO+H2              1.5E13      0.          0.         !(57,-57)
<TSAnG86>!
B1O+B5CH2=>B2CO+2R1H           7.2E13      0.          0.         !(58)
<BAULCH94>!
B1O+B5CH2=B2CO+H2              4.8E13      0.          0.         !(59,-
59)<BAULCH94>!
B1O+R4CH3=HCHO+R1H             8.4E13      0.          0.         !(60,-
60)<BAULCH94>!
B1O+R4CH3=R7CH3O               8.0E15     -2.12     0.6E3         !(61,-
61)<DEAn87nIS>!
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B1O+CH4=R4CH3+R2OH              7.2E8       1.56    8.4E3        !(62,-
62)<BAULCH94>!
B1O+R9C2H=B4CH+B2CO             1.0E13      0.         0.        !(63,-
63)<DAGAUT91>!
B1O+C2H2=B5CH2+B2CO             2.17E06     2.1     1.6E3        !(64,-
64)<BAULCH LEEDS>!
B1O+C2H2=R12CHCOZ+R1H           5.06E06     2.1     1.6E3        !(65,-
65)<BAULCH LEEDS>!
R2OH+R9C2H=C2H2+B1O             1.8E13      0.         0.       !(89,-
89)<TSANG86>! modif MF
B1O+R10C2H3V=R4CH3+B2CO         3.0E13      0.         0.        !(66,-
66)<DAGAUT91>!
B1O+R10C2H3V=CH2COZ+R1H         9.6E13      0.         0.        !(67,-
67)<TSAnG86>!
B1O+C2H4Z=R4CH3+R5CHO           8.1E6       1.88    0.2E3        !(68,-
68)<BAULCH94>!
B1O+C2H4Z=HCHO+B5CH2            4.00E5      1.88    0.2E3        !(69,-
69)<BAULCH94>!
B1O+C2H4Z=CH2COZ+H2             6.6E5       1.88    0.2E3        !(70,-
70)<BAULCH94>!
B1O+C2H4Z=R13CH2CHO+R1H         4.7E6       1.88    0.2E3        !(71,-
71)<BAULCH94>!
B1O+C2H4Z=R2OH+R10C2H3V         1.5E7       1.91    3.7E3        !(72,-
72)<MAHMUD87nIST>!
B1O+R11C2H5=HCHO+R4CH3          1.1E13      0.         0.        !(73,-
73)<BAULCH94>!
B1O+R11C2H5=CH3CHO+R1H          5.5e13      0.         0.        !(74,-
74)<BAULCH94>!
B1O+R11C2H5=C2H4Z+R2OH          3.0E13      0.         0.        !(75,-
75)<DAGAUT91>!
B1O+C2H6=R11C2H5+R2OH           1.0E9       1.5     5.8E3        !(76,-
76)<BAULCH94>!

!****** REACTIONS DE R2OH ******!
R1H+B1O+M=R2OH+M                1.18E19    -1.0      0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R1H+R2OH+M=H2O+M                 5.53E+22   -2.0        0.0
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/
!      N2/0.4/ HE/0.35/
R2OH+H2=R1H+H2O                 1.0E8       1.6     3.3E3        !(79,-
79)<BAULCH94>!
R2OH+B3C=B2CO+R1H              5.0E13      0.         0.        !(80,-
80)<RAnZI94>!
R2OH+B4CH=R5CHO+R1H             3.0E13      0.         0.        !(81,-
81)<DAGAUT91>!
R2OH+B6CH2=HCHO+R1H             3.0E13      0.         0.        !(82,-
82)<TSAnG86>!
R2OH+B5CH2=HCHO+R1H             1.8E13      0.         0.        !(83,-
83)<TSAnG86>!
R2OH+R4CH3=B6CH2+H2O            7.2E13      0.      2.7E3        !(84,-
84)<BAULCH94>!
R2OH+R4CH3(+M)=CH3OH(+M)        6.0E13      0.         0.        !(85,-
85)<BAULCH94>!
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      LOW     /1.4E44     -8.2          0./
      TROE    /0.82      200.        1438./
R2OH+R4CH3=HCHO+H2              3.2E12     -0.53   10.8E3        !(86,-
86)<DAGAUT91>!
R2OH+R4CH3=R7CH3O+R1H           5.7E12     -0.23   13.9E3        !(87,-
87)<DAGAUT91>!
R2OH+CH4=R4CH3+H2O              1.6E7       1.83    2.7E3        !(88,-
88)<BAULCH94>!
!R2OH+R9C2H=C2H2+B1O            1.8E13      0.         0.        !(89,-
89)<TSAnG86>!
R2OH+R9C2H=B5CH2+B2CO           1.8E13      0.         0.        !(90,-
90)<TSAnG86>!
R2OH+R9C2H=R12CHCOZ+R1H         2.0E13      0.         0.        !(91,-
91)<DAGAUT91>!
R2OH+C2H2=R9C2H+H2O             3.385E+07   2.0   14000.0        !(92,-
92)<KONNOV00>!
R2OH+C2H2=CH2COZ+R1H            1.100E+13   0.0    7170.0        !(93,-
93)<KONNOV00>!
R2OH+C2H2=R4CH3+B2CO            4.8E-4      4.     -2.0E3        !(94,-
94)<DAGAUT91>!
R2OH+R10C2H3V=C2H2+H2O          3.0E13      0.         0.        !(95,-
95)<TSAnG86>!
R2OH+R10C2H3V=CH3CHO            3.0E13      0.         0.        !(96,-
96)<TSAnG86>!
R2OH+C2H4Z=R10C2H3V+H2O         2.0E13      0.      5.9E3        !(97,-
97)<BAULCH94>!
R2OH+C2H4Z=R4CH3+HCHO           2.0E12      0.      0.9E3        !(98,-
98)<GLARBORG86>!
R2OH+R11C2H5=C2H4Z+H2O          2.4E13      0.         0.        !(99,-
99)<TSAnG86>!
R2OH+R11C2H5=>R4CH3+R1H+HCHO    2.4E13      0.         0.        !(100)
<TSAnG86>!
R2OH+C2H6=R11C2H5+H2O           7.2E6       2.      0.9E3        !(101,-
101)<BAULCH94>!
R2OH+R2OH=H2O+B1O               1.5E9       1.14    0.1E3        !(102,-
102)<BAULCH94>!

!****** REACTIONS DE H2O ******!
H2O+B4CH=R6CH2OH                5.7E12      0.     -0.8E3        !(103,-
103)<BAULCH94>!
H2O+B6CH2=CH3OH                 1.8E13      0.         0.        !(104,-
104)<TSAnG86>!

!REACTIOnS DE B2CO!
B2CO+R4CH3(+M)=R14CH3CO(+M)     5.0E11      0.      6.9E3        !(105,-
105)<BAULCH94>!
       LOW    /1.1E14      0.      3.8E3/
       TROE   /0.5         1.0      1.0E8/
B2CO+B1O+M=CO2+M                1.54E15     0.0     3.0E3        !(106,-
106)<TSAnG86>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
B2CO+R2OH=CO2+R1H               6.3E6       1.5    -0.5E3        !(107,-
107)<BAULCH94>!
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!REACTIOnS DE R5CHO!
R5CHO+M=R1H+B2CO+M              1.9E17     -1.     17.0E3        !(108,-
108)<WAnG97>!
       H2/2.0/ B2CO/1.5/ CO2/2.0/ H2O/6.0/
R5CHO+R1H=H2+B2CO               9.0E13      0.         0.        !(109,-
109)<BAULCH94>!
R5CHO+R1H=B1O+B5CH2             4.0E13      0.    102.5E3        !(110,-
110)<TSUBOI81nIST>!
R5CHO+B6CH2=R4CH3+B2CO          1.8E13      0.         0.        !(111,-
111)<TSAnG86>!
R5CHO+B5CH2=R4CH3+B2CO          1.8E13      0.         0.        !(112,-
112)<TSAnG86>!
R5CHO+R4CH3=CH4+B2CO            1.2E14      0.         0.        !(113,-
113)<TSAnG86>!
R5CHO+R4CH3=CH3CHO              1.8E13      0.         0.        !(114,-
114)<TSAnG86>!
R4CH3+HCHO=R5CHO+CH4            7.7E-8      6.1    1.97E3        !(115,-
115)<BAULCH94>!
R5CHO+R9C2H=C2H2+B2CO           6.0E13      0.         0.        !(116,-
116)<TSAnG86>!
R5CHO+R10C2H3V=C2H4Z+B2CO       9.0E13      0.         0.        !(117,-
117)<TSAnG86>!
R10C2H3V+HCHO=R5CHO+C2H4Z       5.4E3       2.81    5.9E3        !(118,-
118)<TSAnG86>!
R5CHO+R11C2H5=C2H6+B2CO         1.2E14      0.         0.        !(119,-
119)<TSAnG86>!
R11C2H5+HCHO=R5CHO+C2H6         5.57E3      2.81   5.86E3        !(120,-
120)<TSAnG86>!
R5CHO+B1O=R1H+CO2               3.0E13      0.         0.        !(121,-
121)<BAULCH94>!
R5CHO+B1O=R2OH+B2CO             3.0E13      0.         0.        !(122,-
122)<BAULCH94>!
R5CHO+R2OH=H2O+B2CO             1.1E14      0.         0.        !(123,-
123)<BAULCH94>!
R5CHO+R5CHO=HCHO+B2CO           3.0E13      0.         0.        !(124,-
124)<BAULCH94>!

!****** REACTIONS DE HCHO ******!
HCHO+M=R5CHO+R1H+M              1.40E36    -5.54   96.8E3        !(125,-
125)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+M=H2+B2CO+M                3.26E36    -5.54   96.8E3        !(126,-
126)<BAULCH94>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
HCHO+R1H=R5CHO+H2               1.3E8       1.62    2.1E3        !(127,-
127)<BAULCH94>!
HCHO+B4CH=R13CH2CHO             9.6E13      0.     -0.5E3        !(128,-
128)<BAULCH94average>!
HCHO+B6CH2=R4CH3+R5CHO          1.2E12      0.         0.        !(129,-
129)<TSAnG86>!
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HCHO+B1O=R5CHO+R2OH            4.1E11      0.57    2.7E3         !(130,-
130)<BAULCH94>!
HCHO+R2OH=R5CHO+H2O            7.82E07     1.63  -1.06E3         !MF
Vasudevan Int. J. Chem. Kin. 37(2005)98–109

!****** REACTIONS DE R7CH3O ******!
R7CH3O+M=HCHO+R1H+M             1.55E14     0.00   13.5E3
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R7CH3O+R1H=HCHO+H2             1.8E13      0.          0.         !(133,-
133)<BAULCH94>!
R7CH3O+B6CH2=R4CH3+HCHO        1.8E13      0.          0.         !(134,-
134)<TSAnG86>!
R7CH3O+B5CH2=R4CH3+HCHO        1.8E13      0.          0.         !(135,-
135)<TSAnG86>!
R7CH3O+R4CH3=HCHO+CH4          2.4E13      0.          0.         !(136,-
136)<TSAnG86>!
R7CH3O+CH4=R4CH3+CH3OH         1.6E11      0.       8.8E3         !(137,-
137)<TSAnG86>!
R7CH3O+R9C2H=HCHO+C2H2         2.4E13      0.          0.         !(138,-
138)<TSAnG86>!
R7CH3O+R10C2H3V=HCHO+C2H4Z     2.4E13      0.          0.         !(139,-
139)<TSAnG86>!
R7CH3O+C2H4Z=HCHO+R11C2H5      1.2E11      0.       6.7E3         !(140,-
140)<TSAnG86>!
R7CH3O+R11C2H5=HCHO+C2H6       2.4E13      0.          0.         !(141,-
141)<TSAnG86>!
R7CH3O+C2H6=R11C2H5+CH3OH      2.4E11      0.       7.0E3         !(142,-
142)<TSAnG86>!
R7CH3O+B1O=HCHO+R2OH           1.8E12      0.          0.         !(143,-
143)<BAULCH94>!
R7CH3O+R2OH=HCHO+H2O           1.8E13      0.          0.         !(144,-
144)<TSAnG86>!
R7CH3O+B2CO=R4CH3+CO2          1.6E13      0.      11.7E3         !(145,-
145)<TSAnG86>!
R7CH3O+R5CHO=CH3OH+B2CO        9.1E13      0.          0.         !(146,-
146)<TSAnG86>!
R7CH3O+HCHO=CH3OH+R5CHO        1.0E11      0.       3.0E3         !(147,-
147)<TSAnG86>!
R7CH3O+R7CH3O=CH3OH+HCHO       6.0E13      0.          0.         !(148,-
148)<TSAnG86>!


!****** REACTIONS DE R6CH2OH ******!
R6CH2OH+M=HCHO+R1H+M           1.26E16     0.00   30.0E3         !(149,-
149)<BAULCHLEEDS>!
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
R6CH2OH+R1H=R4CH3+R2OH         9.6E13      0.          0.         !(150,-
150)<TSAnG87>!
R6CH2OH+R1H=HCHO+H2            6.0E12      0.          0.         !(151,-
151)<TSAnG87>!
R6CH2OH+H2=CH3OH+R1H           6.7E5       2.      13.4E3         !(152,-
152)<TSAnG87>!
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R6CH2OH+B6CH2=CH3CHO+R1H       1.8E13      0.          0.         !(153,-
153)<TSAnG87>!
R6CH2OH+B5CH2=C2H4Z+R2OH       2.4E13      0.          0.         !(154,-
154)<TSAnG87>!
R6CH2OH+B5CH2=R4CH3+HCHO       1.2E12      0.          0.         !(155,-
155)<TSAnG87>!
R6CH2OH+R4CH3=C2H5OH          1.2E13      0.          0.         !(156,-
156)<TSAnG87>!
R6CH2OH+R4CH3=CH4+HCHO         2.4E12      0.          0.         !(157,-
157)<TSAnG87>!
R6CH2OH+CH4=CH3OH+R4CH3        21.7        3.1    16.2E3         !(158,-
158)<TSAnG87>!
R6CH2OH+R9C2H=C2H2+HCHO        4.8E13      0.          0.         !(159,-
159)<TSAnG87>!
!la constante de vitesse du processus 159 est globalisee!
!R6CH2OH+R9C2H=C3H3+R2OH       1.2E13      0.          0.         !(159a,-
159a)<TSAnG87>!
!R6CH2OH+R9C2H=C2H2+HCHO       3.6E13      0.          0.         !(159b,-
159b)<TSAnG87>!
R6CH2OH+C2H2=R10C2H3V+HCHO     7.2E11      0.       9.0E3         !(160,-
160)<TSAnG87>!
R6CH2OH+R10C2H3V=C2H4Z+HCHO    4.2E13      0.          0.         !(161,-
161)<TSAnG87>!
!La constante de vitesse  du processus 161 est globalisee!
R6CH2OH+R11C2H5=C2H4Z+CH3OH    2.4E12      0.          0.         !(162,-
162)<TSAnG87>!
R6CH2OH+R11C2H5=C2H6+HCHO      2.4E12      0.          0.         !(163,-
163)<TSAnG87>!
R6CH2OH+C2H6=CH3OH+R11C2H5     199.        3.     14.0E3          !(164,-
164)<TSAnG87>!
R6CH2OH+B1O=HCHO+R2OH          4.2E13      0.          0.         !(165,-
165)<TSAnG87>!
R6CH2OH+R2OH=H2O+HCHO          2.4E13      0.          0.         !(166,-
166)<TSAnG87>!
!attention (167) metatheses dans les reactions de CH3OH!
!R6CH2OH+H2O=CH3OH+R2OH        1.6E14      0.     26.3E3          !(167,-
167)<TSUBOI81nIST>!
R6CH2OH+R5CHO=CH3OH+B2CO       1.2E14      0.          0.         !(168,-
168)<TSAnG87>!
R6CH2OH+R5CHO=HCHO+HCHO        1.8E14      0.          0.         !(169,-
169)<TSAnG87>!
R6CH2OH+HCHO=CH3OH+R5CHO       5.5E3       2.8     5.9E3          !(170,-
170)<TSAnG87>!
R6CH2OH+R7CH3O=CH3OH+HCHO      2.4E13      0.          0.         !(171,-
171)<TSAnG87>!
R6CH2OH+R6CH2OH=CH3OH+HCHO     1.4E13      0.          0.         !(172,-
172)<TSAnG87>!
!la constante de vitesse du processus 172 est globalisee!
!R6CH2OH+R6CH2OH=CH3OH+HCHO    4.8E12      0.          0.         !(172a,-
172a)<TSAnG87>!
!R6CH2OH+R6CH2OH=HOCH2CH2OH    9.6E12      0.          0.         !(172b,-
172b)<TSAnG87>!

!****** REACTIONS DE CH3OH ******!
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```
CH3OH+R1H=R4CH3+H2O            2.0E14      0.      5.3E3        !(173,-
173)<HIDAKA89nIST>!
CH3OH+R1H=R7CH3O+H2            4.2E6       2.1     4.9E3        !(174,-
174)<TSAnG87>!
CH3OH+B6CH2=R6CH2OH+R4CH3      1.5E12      0.        0.         !(175,-
175)<TSAnG87>!
CH3OH+B5CH2=R4CH3+R6CH2OH      31.9        3.2     7.2E3        !(176,-
176)<TSAnG87>!
CH3OH+B5CH2=R4CH3+R7CH3O       14.4        3.1     6.9E3        !(177,-
177)<TSAnG87>!
CH3OH+R9C2H=C2H2+R6CH2OH       6.0E12      0.        0.         !(178,-
178)<TSAnG87>!
CH3OH+R9C2H=C2H2+R7CH3O        1.2E12      0.        0.         !(179,-
179)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R6CH2OH   31.9        3.2     7.2E3        !(180,-
180)<TSAnG87>!
CH3OH+R10C2H3V=C2H4Z+R7CH3O    14.4        3.1     6.9E3        !(181,-
181)<TSAnG87>!
CH3OH+B1O=R6CH2OH+R2OH         3.4E13      0.      5.5E3         !(182,-
182)<GROTHEER81nIST>!
CH3OH+B1O=R7CH3O+R2OH          1.0E13      0.      4.7E3        !(183,-
183)<WARnATZ84>!
!modification des metatheses avec OH!
!CH3OH+R2OH=R7CH3O+H2O         1.0E13      0.      1.7E3        !(184,-
184)<WARnATZ84>!
CH3OH+R2OH=R6CH2OH+H2O         3.1E06      2.     -3.4E2        !(184a,-
184a)<Atkinson86>85%!
CH3OH+R2OH=R7CH3O+H2O          5.4E05      2.     -3.4E2        !(184b,-
184b)<Atkinson86>15%!
CH3OH+R7CH3O=CH3OH+R6CH2OH     3.0E11      0.      4.1E3        !(185,-
185)<TSAnG87>!

!****** REACTIONS DE R12CHCOD ******!
R12CHCOZ+M=B4CH+B2CO+M         6.0E15      0.     58.8E3        !(186,-
186)<DAGAUT91>!
R12CHCOZ+R1H=B5CH2+B2CO        1.5E14      0.        0.         !(187a,-
187a)<BAULCH94>!
R12CHCOZ+R1H=B6CH2+B2CO        1.3E14      0.        0.         !(187b,-
187b)<PEETERS97>!
R12CHCOZ+B5CH2=R9C2H+HCHO      1.0E13      0.      2.0E3        !(188,-
188)<DAGAUT91>!
R12CHCOZ+B5CH2=R10C2H3V+B2CO   3.0E13      0.        0.         !(189,-
189)<DAGAUT91>!
R12CHCOZ+B1O=>B2CO+B2CO+R1H    9.6E13      0.        0.         !
(190)<BAULCH94>!
R12CHCOZ+R2OH=>R5CHO+B2CO+R1H  1.0E13      0.        0.         !
(191)<DAGAUT91>!


!****** REACTIONS DE CH2COD ******!
CH2COZ+M=B6CH2+B2CO+M          6.57E15     0.0    57.6E3        !(192,-
192)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
```

```
CH2COZ+M=R12CHCOZ+R1H+M        2.7E17      0.     87.0E3        !(193,-
193)<FRAnK86nIST>!
       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
CH2COZ+R1H=R4CH3+B2CO          1.8E13      0.      3.4E3        !(194,-
194)<BAULCH94>!
CH2COZ+R1H=R12CHCOZ+H2         5.0E13      0.      8.0E3        !(195,-
195)<DAGAUT91>!
CH2COZ+B5CH2=C2H4Z+B2CO        1.3E14      0.         0.        !(196,-
196)<CAnOSA-MAS84nIST>!
CH2COZ+B1O=B5CH2+CO2           1.8E12      0.      1.3E3        !(197,-
197)<DAGAUT91>!
CH2COZ+B1O=R12CHCOZ+R2OH       1.0E13      0.      8.0E3        !(198,-
198)<DAGAUT91>!
CH2COZ+R2OH=R12CHCOZ+H2O       7.5E12      0.      2.0E3        !(199,-
199)<DAGAUT91>!
!CH2COZ+R2OH=R5CHO+HCHO        2.8E13      0.        0.         !(200,-
200)<VAnDOOREn77nIST>!
CH2COZ+R2OH=R4CH3+CO2          2.52E12     0.         0.        !(200a,-
200a)<BAULCH LEEDS>!
CH2COZ+R2OH=R6CH2OH+B2CO       4.68E12     0.         0.        !(200b,-
200b)<BAULCH LEEDS>!


!****** REACTIONS DE R14CH3CO ******!
R14CH3CO+R1H=R4CH3+R5CHO        9.6E13      0.         0.        !(201,-
201)<TSAnG86>!
R14CH3CO+B6CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(202,-
202)<TSAnG86>!
R14CH3CO+B5CH2=R4CH3+CH2COZ     1.8E13      0.         0.        !(203,-
203)<TSAnG86>!
R14CH3CO+B1O=R4CH3+CO2          9.6E12      0.         0.        !(204,-
204)<TSAnG86>!
R14CH3CO+R2OH=CH2COZ+H2O        1.2E13      0.         0.        !(205,-
205)<TSAnG86>!
R14CH3CO+R2OH=>R4CH3+B2CO+R2OH  3.0E13      0.         0.        !
(206)<TSAnG86>!
R14CH3CO+R5CHO=CH3CHO+B2CO      9.0E12      0.         0.        !(207,-
207)<TSAnG86>!
R14CH3CO+HCHO=CH3CHO+R5CHO      1.8E11      0.     12.9E3        !(208,-
208)<TSAnG86>!
R14CH3CO+R7CH3O=CH3OH+CH2COZ    6.0E12      0.         0.        !(209,-
209)<TSAnG86>!
R14CH3CO+R7CH3O=HCHO+CH3CHO     6.0E12      0.         0.        !(210,-
210)<TSAnG86>!
R14CH3CO+CH3OH=CH3CHO+R6CH2OH   4.85E3      3.     12.3E3        !(211,-
211)<TSAnG87>!
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 1.2E13      0.         0.        !(212,-
212)<TSAnG86>!

!****** REACTIONS DE R13CH2CHO ******!
!R13CH2CHO=R14CH3CO               1.0E13      0.      47.0E3          !
(213,-213)<COLKET75nIST>!
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```
!R13CH2CHO=R1H+CH2COZ              1.6E13      0.      35.0E3          !
(214,-214)<COLKET75nIST>!
R13CH2CHO=R4CH3+B2CO                 2.93E12     0.29    40.3E3!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.
R13CH2CHO=R1H+CH2COZ                1.43E15     -0.15   45.6E3 !at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.


!****** REACTIONS DE CH3CHO ******!
!CH3CHO+R1H=H2+R14CH3CO            4.0E13      0.       4.2E3          !
(215,-215)<WARnATZ84>!
!CH3CHO+R4CH3=R14CH3CO+CH4         2.0E-6      5.6      2.5E3          !
(216,-216)<BAULCH94>!
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO    8.1E10      0.       3.7E3          !
(217,-217)<SCHERZER87>!
!CH3CHO+R11C2H5=C2H6+R14CH3CO      1.3E12      0.       8.5E3          !
(218,-218)<HOHLEIn70>!
!CH3CHO+B1O=R14CH3CO+R2OH          1.4E13      0.       2.3E3          !
(219,-219)<CAVAnAGH90>!
!CH3CHO+R2OH=R14CH3CO+H2O          4.2E12      0.       0.5E3          !
(220,-220)<CAVAnAGH90>!
!CH3CHO+R7CH3O=R14CH3CO+CH3OH      2.4E11      0.       1.8E3          !
(221,-221)<CAVAnAGH90>!
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 2.5E7       0.         0.           !
(222,-222)<SCHUCHMAnn70nIST>!

!****** REACTIONS DE C2H4O# ******!
C2H4O#3=CH4+B2CO                    1.2E13      0.      57.2E3   !(223,-
223)<LIFSHITZ83nIST>!
C2H4O#3=CH3CHO                      7.3E13      0.      57.2E3   !(224,-
224)<LIFSHITZ83nIST>!
C2H4O#3=R4CH3+R5CHO                 3.6E13      0.      57.2E3   !(225,-
225)<LIFSHITZ83nIST>!
C2H4O#3+R1H=H2+R13CH2CHO            2.0E13      0.       8.3E3   !(226,-
226)<LIFSHITZ83nIST*>!
C2H4O#3+R1H=H2O+R10C2H3V            5.0E9       0.       5.0E3   !(227,-
227)<LIFSHITZ83nIST>!
C2H4O#3+R1H=C2H4Z+R2OH              9.5E10      0.       5.0E3   !(228,-
228)<LIFSHITZ83nIST>!
C2H4O#3+R4CH3=CH4+R13CH2CHO         1.1E12      0.      11.8E3   !(229,-
229)<BALDWIn84nIST*>!
C2H4O#3+R4CH3=R11C2H5+HCHO          1.4E11      0.       7.6E3   !(230,-
230)<RAnZI94>!
C2H4O#3+R4CH3=C2H4Z+R7CH3O          1.5E10      0.       7.6E3   !(231,-
231)<RAnZI94>!
C2H4O#3+R9C2H=C2H2+R13CH2CHO        1.2E12      0.       9.8E3   !(232,-
232)<RAnZI94>!
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO    2.0E12      0.       9.3E3   !(233,-
233)<RAnZI94>!
C2H4O#3+R11C2H5=C2H6+R13CH2CHO      6.8E11      0.      11.4E3   !(234,-
234)<RAnZI94>!
C2H4O#3+B1O=R2OH+R13CH2CHO          1.9E12      0.       5.2E3   !(235,-
235)<BOGAn78nIST>!
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C2H4O#3+R2OH=H2O+R13CH2CHO         1.8E13      0.       3.6E3    !(236,-
236)<BALDWIn84nIST*>!
C2H4O#3+R5CHO=HCHO+R13CH2CHO       3.7E12      0.      15.8E3    !(237,-
237)<RAnZI94>!
C2H4O#3+R7CH3O=CH3OH+R13CH2CHO     1.3E12      0.       5.8E3    !(238,-
238)<RAnZI94>!
C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO    8.4E11      0.      13.4E3    !(239,-
239)<RAnZI94>!
C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO  4.0E12      0.      17.5E3    !(240,-
240)<RAnZI94>!
C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO 6.8E11      0.      15.4E3    !(241,-
241)<RAnZI94>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!

!****** REACTIONS DE R15C2H5O ******!

!****** REACTIONS DE C2H5OH ******!

!Voir Plus bas meca 10a Luc Sy Tran

!****** REACTIONS DE O2 ******!
B1O+B1O+M=O2+M                  5.40E13     0.   -1.79E3    !(244,-
244)<BAULCH94>!
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!      N2/0.4/ HE/0.35/
O2+R1H=R2OH+B1O                 9.8E13      0.     14.8E3    !(245,-
245)<BAULCH94>!
!O2+R1H+M=R3OOH+M                2.10E18    -0.8    0.00      !(246,-
246)<baseLeeds>!
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H+H2O=R3OOH+H2O            6.90E15    0.0    -2.10E3    !(246,-
246bis)<base Leeds>!

O2+R1H(+M)=R3OOH(+M)            4.52E13     0.       0.           !(246,-
246)<COBOS85>!
               LOW   /1.8E18     -0.8       0.00/                     !k0
BAULCH94!
               TROE  /0.5         1.0      1.0E8/
        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/
!        N2/0.4/ HE/0.35/
!O2+R1H(+H2O)=R3OOH(+H2O)        1.63E14     0.       761.    !(246b,-
246b)<COBOS85>!
O2+R1H(+H2O)=R3OOH(+H2O)        4.52E13     0.         0.    !(246b,-
246b)<BAULCH94>!
               LOW   /6.9E15     0.0      -2080/
               TROE  /0.45       1.0      1.0E8/
O2+B3C=B2CO+B1O                1.2E14      0.         0.     !(247,-
247)<RAnZI94>!
O2+B4CH=R5CHO+B1O               3.3E13      0.         0.    !(248,-
248)<DAGAUT91>!
O2+B4CH=B2CO+R2OH               3.2E13      0.         0.    !(249,-
249)<PEETERS97>!
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```
O2+B6CH2=>B2CO+R2OH+R1H          3.1E12      0.          0.    !
(250)<BAULCH94>!
O2+B5CH2=R5CHO+R2OH              4.3E10      0.      -0.5E3    !(251,-
251)<DAGAUT91>!
O2+B5CH2=CO2+H2                  6.9E11      0.       0.5E3    !(252,-
252)<DAGAUT91>!
O2+B5CH2=>CO2+R1H+R1H            1.6E12      0.       1.0E3    !
(253)<DAGAUT91>!
O2+B5CH2=B2CO+H2O                1.9E10      0.      -1.0E3    !(254,-
254)<DAGAUT91>!
O2+B5CH2=>B2CO+R2OH+R1H          8.6E10      0.      -0.5E3    !
(255)<DAGAUT91>!
O2+B5CH2=HCHO+B1O                1.0E14      0.       4.5E3    !(256,-
256)<DAGAUT91>!
O2+R4CH3(+M)=R8CH3OO(+M)         7.8E8       1.2         0.   !(257,-
257)<BAULCH94>!
                     LOW   /5.6E25     -3.3        0./
                     TROE  /0.36        1.0      1.0E8/
O2+R4CH3=R7CH3O+B1O              1.3E14      0.      31.3E3    !(258,-
258)<BAULCH94>!
!O2+R4CH3=R7CH3O+B1O             1.6E13      0.      31.4E3    !(258,-
258)<HWAnG&RABInOVITCH99>!

O2+R4CH3=HCHO+R2OH               3.0E30     -4.69    36.6E3    !(259,-
259)<DAGAUT91>!
O2+CH4=R4CH3+R3OOH               4.0E13      0.      56.7E3    !(260,-
260)<BAULCH94>!
O2+R9C2H=B2CO+R5CHO              3.8E13     -0.16        0.   !(261,-
261)<TIESEMAnn97/TSAnG86>!
O2+R9C2H=R12CHCOZ+B1O            9.0E12     -0.16        0.   !(262,-
262)<TIESEMAnn97/TSAnG86>!
O2+C2H2=R9C2H+R3OOH              1.2E13      0.      74.5E3    !(263,-
263)<TSAnG86>!
!O2+C2H2=R12CHCOZ+R2OH           2.0E8       1.5     30.1E3    !(264,-
264)<DAGAUT91>!
O2+C2H2=R5CHO+R5CHO              7.0E7       1.8     30.6E3    !(264,-
264)<BEnSOn95>!

!O2+R10C2H3V=C2H2+R3OOH          1.2E11      0.          0.    !(265,-
265)<TSAnG86>!

!O2+R10C2H3V=C2H2+R3OOH          1.6E14     -0.83     2.5E3    !(265,-
265)<WAnG97>!
!at 760 Torr
!O2+R10C2H3V=HCHO+R5CHO          8.6E21     -2.97     3.3E3    !(266a,-
266a)<WAnG97>!
!O2+R10C2H3V=B1O+R13CH2CHO       1.2E13     -0.12     1.7E3    !(266b,-
266b)<WAnG97>!
!at 20-90 Torr
!O2+R10C2H3V=HCHO+R5CHO          1.6E21     -2.78     2.5E3    !(266a,-
266a)<WAnG97>!
!O2+R10C2H3V=B1O+R13CH2CHO       2.5E12      0.057    0.9E3    !(266b,-
266b)<WAnG97>!
```

```
O2+R10C2H3V=C2H2+R3OOH          1.34E6      1.61    -0.4E3   !(265,-
265)<MEBEL nIST>!
O2+R10C2H3V=HCHO+R5CHO          4.5E16     -1.39     1.0E3   !(266a,-
266a)<MEBEL nIST>!
O2+R10C2H3V=B1O+R13CH2CHO       3.3E11     -0.29       10.   !(266b,-
266b)<MEBEL nIST>!

O2+C2H4Z=R10C2H3V+R3OOH         4.2E13      0.      57.4E3   !(267,-
267)<TSAnG86>!
O2+R11C2H5=R17C2H5OO           2.2E10      0.77    -0.6E3    !(268,-
268)<WAGnER90>!
O2+R11C2H5=C2H4Z+R3OOH          8.4E11      0.       3.9E3   !(269,-
269)<TSAnG86>!
O2+R11C2H5=R15C2H5O+B1O         1.2E13     -0.2     27.9E3   !(270,-
270)<BOZZELLI90nIST>!
O2+R11C2H5=CH3CHO+R2OH          6.0E10      0.       6.9E3   !(271,-
271)<TSAnG86>!
O2+C2H6=R11C2H5+R3OOH           6.0E13      0.      51.7E3   !(272,-
272)<BAULCH94>!
O2+R2OH=R3OOH+B1O               2.2E13      0.      52.5E3   !(273,-
273)<TSAnG86>!
O2+B2CO=CO2+B1O                 2.5E12      0.      47.7E3   !(274,-
274)<TSAnG86>!
!O2+R5CHO=B2CO+R3OOH            5.1E13      0.       1.7E3   !(275,-
275)<TSAnG86>!
O2+R5CHO=B2CO+R3OOH             7.6E12      0.      0.41E3   !(275,-
275)<TIMOnEn88>!
O2+HCHO=R5CHO+R3OOH             2.0E13      0.      38.8E3   !(276,-
276)<TSAnG86)!
O2+R7CH3O=HCHO+R3OOH            2.2E10      0.       1.7E3   !(277,-
277)<BAULCH94>!
O2+R6CH2OH=HCHO+R3OOH           1.2E12      0.          0.   !(278,-
278)<TSAnG87>!
O2+CH3OH=R6CH2OH+R3OOH          2.0E13      0.      44.9E3   !(279,-
279)<TSAnG87>!
O2+R12CHCOZ=>B2CO+B2CO+R2OH     1.5E12      0.       2.5E3   !(280)
<DAGAUT91>!
!O2+CH2COZ=HCHO+CO2             1.0E8       0.          0.   !(281,-
281)<DAGAUT91>!bizarre
O2+R14CH3CO=R18CH3COOO         2.4E12      0.           0.    !(282,-
282)<COX90>!
O2+R13CH2CHO=>HCHO+R2OH+B2CO    5.9E9       0.      -1.4E3   !(283)
<COX90>!
O2+R13CH2CHO=CH2COZ+R3OOH       1.0E10      0.      -1.4E3   !(284,-
284)<COX90>!
O2+CH3CHO=R14CH3CO+R3OOH        5.0E13      0.      36.4E3   !(285,-
285)<COX90>!
! ajout demande par Laetitia le 25 Avril 95
O2+CH3CHO=R13CH2CHO+R3OOH       1.0E13      0.5     46.0E3   !(285',-
285)<Ranzi94>!
O2+C2H4O#3=R3OOH+R13CH2CHO      5.0E13      0.      48.0E3   !(286,-
286)<RAnZI94>!
!O2+R15C2H5O=CH3CHO+R3OOH        6.0E10      0.       1.7E3  !(287,-
287)<BAULCH94>!
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!****** REACTIONS DE R3OOH ******!
R3OOH+R1H=H2+O2                 4.3E13      0.      1.4E3  !(288,-
288)<BAULCH94>!
R3OOH+R1H=2R2OH                 1.7E14      0.      0.9E3  !(289,-
289)<BAULCH94>!
R3OOH+R1H=H2O+B1O               3.0E13      0.      1.7E3  !(290,-
290)<BAULCH94>!
R3OOH+B6CH2=HCHO+R2OH           3.0E13      0.         0.  !(291,-
291)<TSAnG86>!
R3OOH+B5CH2=HCHO+R2OH           1.8E13      0.         0.  !(292,-
292)<TSAnG86>!
R3OOH+R4CH3=R7CH3O+R2OH         1.8E13      0.         0.  !(293,-
293)<BAULCH94>!
!R3OOH+R4CH3=R7CH3O+R2OH        4.0E13      0.      5.0E3  !(293,-
293)<DAGAUT>
R3OOH+CH4=R4CH3+H2O2            9.0E12      0.     24.6E3  !(294,-
294)<BAULCH94>!
R3OOH+R9C2H=R12CHCOZ+R2OH       1.8E13      0.         0.  !(295,-
295)<TSAnG86>!
R3OOH+C2H2=CH2COZ+R2OH          6.0E9       0.      8.0E3  !(296,-
296)<TSAnG86>!
!incertitude au moins un facteur 10
R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO 3.0E13      0.         0.  !(297)
<TSAnG86>!
R3OOH+C2H4Z=CH3CHO+R2OH         6.0E9       0.      7.9E3  !(298,-
298)<TSAnG86>!
R3OOH+C2H4Z=C2H4O#3+R2OH        2.2E12      0.     17.2E3  !(299,-
299)<BAULCH94>!
R3OOH+R11C2H5=>R4CH3+HCHO+R2OH  2.4E13      0.         0.  !(300)
<TSAnG86>!
R3OOH+R11C2H5=C2H4Z+H2O2        3.0E11      0.         0.  !(301,-
301)<TSAnG86>!
R3OOH+C2H6=R11C2H5+H2O2         1.3E13      0.     20.4E3  !(302,-
302)<BAULCH94>!
R3OOH+R2OH=H2O+O2               2.9E13      0.     -0.5E3  !(303,-
303)<BAULCH94>!
R3OOH+B2CO=CO2+R2OH             1.57E05     2.18   17.9E3  !MF Wang, J.
Phys. Chem. A 111(2007)4031 - 4042
R3OOH+R5CHO=>R2OH+R1H+CO2       3.0E13      0.         0.  !(305)
<TSAnG86>!
R3OOH+HCHO=R5CHO+H2O2           3.0E12      0.     13.0E3  !(306,-
306)<BAULCH94>!
R3OOH+R7CH3O=HCHO+H2O2          3.0E11      0.         0.  !(307,-
307)<TSAnG86>!
R3OOH+R6CH2OH=HCHO+H2O2         1.2E13      0.         0.  !(308,-
308)<TSAnG87>!
R3OOH+CH3OH=R6CH2OH+H2O2        9.6E10      0.     12.6E3  !(309,-
309)<TSAnG87>!
R3OOH+R14CH3CO=>R4CH3+CO2+R2OH  3.0E13      0.         0.  !
(310)<TSAnG86>!
R3OOH+CH3CHO=R14CH3CO+H2O2      1.0E12      0.     10.0E3  !(311,-
311)<CAVAnAGH90>!
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R3OOH+C2H4O#3=H2O2+R13CH2CHO    1.6E12      0.     15.0E3  !(312,-
312)<RAnZI94>
R3OOH+R3OOH=H2O2+O2             1.3E11      0.    -1.63E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE
R3OOH+R3OOH=H2O2+O2             4.2E14      0.    11.98E3  !(313,-
313)<BAULCH 94>!
     DUPLICATE

!****** REACTIONS DE H2O2 ******!
!R2OH+R2OH(+ M)=>H2O2 (+ M)     7.23E13    -0.37    0.00
!       O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /5.53E19  -0.76     0.00 /
!        TROE /0.5 1 1.E8/
!H2O2(+M)=>R2OH+R2OH(+M)         3.00E14     0.00    48.5E3
!        O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/
!!        N2/0.4/ HE/0.35/
!        LOW  /3.0E17   0.0     45.5E3/
!       TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601
H2O2(+M)=R2OH+R2OH(+M)        1.99E12     0.9    4.8749E4 !<BAULCH94>!
          AR/0.68/ O2/0.79/ N2/1.00/ CO2/1.06/ H2O/5.1/ H2O2/5.2/
        LOW  /3.65e24   -2.3   4.8749E4/
        TROE /0.43 1 1.E8/

H2O2+R1H=H2+R3OOH               1.7E12      0.      3.7E3   !(315,-
315)<BAULCH94>!
H2O2+R1H=H2O+R2OH               1.0E13      0.      3.6E3   !(316,-
316)<BAULCH94>!
H2O2+B6CH2=R7CH3O+R2OH          3.0E13      0.         0.   !(317,-
317)<TSAnG86>!
H2O2+R10C2H3V=C2H4Z+R3OOH       1.2E10      0.     -0.6E3   !(318,-
318)<TSAnG86>!
H2O2+B1O=R2OH+R3OOH             6.6E11      0.      4.0E3   !(319,-
319)<BAULCH94>!
H2O2+R2OH=H2O+R3OOH             7.8E12      0.      1.3E3   !(320,-
320)<BAULCH94>!

!****** REACTIONS DE CO2 ******!
CO2+B5CH2=HCHO+B2CO             2.3E10      0.         0.   !(321,-
321)<TSAnG86>!

!****** REACTIONS DE R8CH3OO ******!
R8CH3OO=HCHO+R2OH                 1.5E13      0.     47.0E3 !(322,-
322)<RAnZI94>!
R8CH3OO+R1H=R7CH3O+R2OH           9.6E13      0.         0. !(323,-
323)<TSAnG86>!
R8CH3OO+H2=CH3OOH+R1H             3.0E13      0.     26.0E3 !(324,-
324)<TSAnG86>!
R8CH3OO+B6CH2=HCHO+R7CH3O         1.8E13      0.         0. !(325,-
325)<TSAnG86>!
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R8CH3OO+B5CH2=HCHO+R7CH3O          1.8E13      0.          0. !(326,-
326)<TSAnG86>!
R8CH3OO+R4CH3=R7CH3O+R7CH3O        5.0E12      0.      -1.4E3 !(327,-
327)<CAVAnAGH90>!
R8CH3OO+CH4=CH3OOH+R4CH3           1.8E11      0.      18.5E3 !(328,-
328)<TSAnG86>!
R8CH3OO+R9C2H=R7CH3O+R12CHCOZ      2.4E13      0.          0. !(329,-
329)<TSAnG86>!
!R8CH3OO+C2H2=CH3OOH+R9C2H          5.6E11      0.      24.5E3 !(330,-
330)<RAnZI94>! MF car i<<0
R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO 2.4E13      0.          0. !(331,-
331)<TSAnG86*>!
!* assuming that C2H3O decompose rapidly to R13CH2CHO!
R8CH3OO+C2H4Z=R7CH3O+C2H4O#3       1.1E15      0.      20.0E3 !(332,-
332)<nIKISHA81/MOSHKInA80nIST>!
R8CH3OO+C2H4Z=CH3OOH+R10C2H3V      3.9E12      0.      24.5E3 !(333,-
333)<RAnZI94>!
R8CH3OO+R11C2H5=R7CH3O+R15C2H5O    2.4E13      0.          0. !(334,-
334)<TSAnG86>!
R8CH3OO+C2H6=CH3OOH+R11C2H5        2.9E11      0.      14.9E3 !(335,-
335)<TSAnG86>!
R8CH3OO+B1O=R7CH3O+O2              3.6E13      0.          0. !(336,-
336)<TSAnG86>!
R8CH3OO+R2OH=CH3OH+O2              6.0E13      0.          0. !(337,-
337)<TSAnG86>!
R8CH3OO+R2OH=R7CH3O+R3OOH          3.0E12      0.          0. !(338,-
338)<RAnZI94>!
R8CH3OO+B2CO=R7CH3O+CO2            1.0E14      0.      24.0E3 !(339,-
339)<RAnZI94>!
R8CH3OO+R5CHO=>R7CH3O+R1H+CO2      3.0E13      0.          0. !(340)
<TSAnG86>!
R8CH3OO+HCHO=CH3OOH+R5CHO          1.0E12      0.      12.1E3 !(341,-
341)<CAVAnAGH90>!
R8CH3OO+R7CH3O=HCHO+CH3OOH         3.0E11      0.          0. !(342,-
342)<TSAnG86>!
R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO 1.2E13      0.          0. !
(343)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R6CH2OH       1.8E12      0.      13.7E3 !(344,-
344)<TSAnG87>!
R8CH3OO+CH3OH=CH3OOH+R7CH3O        2.8E11      0.      18.8E3 !(345,-
345)<RAnZI94>!
R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ     1.7E12      0.      27.0E3 !(346,-
346)<RAnZI94>!
R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O  2.4E13      0.          0. !(347,-
347)<TSAnG86>!
R8CH3OO+CH3CHO=CH3OOH+R14CH3CO     1.0E12      0.      12.1E3 !(348,-
348)<CAVAnAGH90>!
R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO    1.7E12      0.      19.2E3 !(349,-
349)<RAnZI94>!
R8CH3OO+C2H4O#3=CH3OOH+R13CH2CHO   2.2E12      0.      16.0E3 !(350,-
350)<RAnZI94>!
R8CH3OO+R3OOH=CH3OOH+O2            2.5E11      0.      -1.6E3 !(351,-
351)<BAULCH94>!
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R8CH3OO+R3OOH=>O2+HCHO+H2O         5.0E10      0.          0. !
(352)<RAnZI94>!
R8CH3OO+H2O2=CH3OOH+R3OOH          2.4E12      0.       9.9E3 !(353,-
353)<TSAnG86>!
R8CH3OO+R8CH3OO=CH3OH+HCHO+O2      2.5E10      0.      -0.8E3 !(354,-
354)<BAULCH94>!
R8CH3OO+R8CH3OO=R7CH3O+R7CH3O+O2   2.5E10      0.      -0.8E3 !(355,-
355)<BAULCH94>!

!****** REACTIOnS DE CH3OOH ******!
CH3OOH=R7CH3O+R2OH                 6.0E14      0.      42.3E3 !(356,-
356)<BAULCH94>!
CH3OOH+B1O=R8CH3OO+R2OH            2.0E13      0.       4.8E3 !(357,-
357)<BAULCH94average>!
CH3OOH+R2OH=H2O+R8CH3OO            1.8E12      0.    -0.37E3 !(358,-
358)<BAULCH94average>!
CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO     1.5E11      0.       6.5E3 !
(359)<RAnZI94>!

!****** REACTIOnS DE R17C2H5OO ******!
R17C2H5OO=R16C2H4OOH                 4.2E12      0.      36.9E3 !(360,-
360)<HUGHES93>!
R17C2H5OO+H2=C2H5OOH+R1H             7.9E12      0.      21.0E3 !(361,-
361)<RAnZI94>!
R17C2H5OO+R4CH3=R15C2H5O+R7CH3O      2.0E12      0.      -1.2E3 !(362,-
362)<RAnZI94>!
R17C2H5OO+CH4=C2H5OOH+R4CH3          3.9E12      0.      24.0E3 !(363,-
363)<RAnZI94>!
R17C2H5OO+C2H2=C2H5OOH+R9C2H         5.6E11      0.      24.4E3 !(364,-
364)<RAnZI94>!
R17C2H5OO+C2H4Z=C2H5OOH+R10C2H3V     3.9E12      0.      24.4E3 !(365,-
365)<RAnZI94>!
R17C2H5OO+C2H4Z=R15C2H5O+C2H4O#3     2.3E16      0.      21.9E3 !(366,-
366)<MOSHKInA80nIST>!
R17C2H5OO+C2H6=C2H5OOH+R11C2H5       5.1E12      0.      19.5E3 !(367,-
367)<RAnZI94>!
R17C2H5OO+H2O=C2H5OOH+R2OH           5.6E12      0.      30.6E3 !(368,-
368)<RAnZI94>!
R17C2H5OO+B2CO=CO2+R15C2H5O          1.0E14      0.      24.0E3 !(369,-
369)<RAnZI94>!
R17C2H5OO+HCHO=C2H5OOH+R5CHO         4.5E12      0.      14.4E3 !(370,-
370)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R7CH3O       2.8E11      0.      18.4E3 !(371,-
371)<RAnZI94>!
R17C2H5OO+CH3OH=C2H5OOH+R6CH2OH      2.8E12      0.      19.5E3 !(372,-
372)<RAnZI94>!
R17C2H5OO+CH2COZ=C2H5OOH+R12CHCOZ    1.7E12      0.      24.4E3 !(373,-
373)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R14CH3CO    3.9E12      0.      14.4E3 !(374,-
374)<RAnZI94>!
R17C2H5OO+CH3CHO=C2H5OOH+R13CH2CHO   1.7E12      0.      19.5E3 !(375,-
375)<RAnZI94>!
R17C2H5OO+C2H4O#3=C2H5OOH+R13CH2CHO  2.2E12       0.      16.3E3 !(376,-
376)<RAnZI94>!
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R17C2H5OO+R3OOH=O2+C2H5OOH          3.9E11      0.     -1.3E3 !(377,-
377)<BAULCH89>!
!Rate constant measured between 240 and 380K!
R17C2H5OO+H2O2=C2H5OOH+R3OOH        4.5E11      0.     10.8E3 !(378,-
378)<RAnZI94>!
R17C2H5OO+R8CH3OO=>R15C2H5O+R7CH3O+O2  2.0E11      0.         0. !
(379)<RAnZI94>!
R17C2H5OO+CH3OOH=C2H5OOH+R8CH3OO    1.1E12      0.     16.3E3 !(380,-
380)<RAnZI94>!
R17C2H5OO+R17C2H5OO=2R15C2H5O+O2    4.1E10      0.      0.2E3 !(381,-
381)<LIGHTFOOT92>!
R17C2H5OO+R17C2H5OO=C2H5OH+CH3CHO+O2  1.8E10      0.       0.2E3 !(382,-
382)<LIGHTFOOT92>!

!****** REACTIONS DE R16C2H4OOH ******!
R16C2H4OOH=C2H4O#3+R2OH             1.5E11      0.     20.0E3 !(383,-
383)<RAnZI94>!
R16C2H4OOH=R6CH2OH+HCHO             2.5E13      0.     27.5E3 !(384,-
384)<RAnZI94>!
R16C2H4OOH=C2H4Z+R3OOH              2.0E13      0.     23.5E3 !(385,-
385)<RAnZI94>!

!****** REACTIONS DE C2H5OOH ******!
C2H5OOH=R15C2H5O+R2OH                4.0E15      0.     42.9E3 !(386,-
386)<BAULCH94>!
C2H5OOH+R1H=>CH3CHO+R2OH+H2          3.2E13      0.      7.7E3 !
(387)<RAnZI94>!
C2H5OOH+R4CH3=>CH3CHO+R2OH+CH4       5.7E11      0.      8.7E3 !
(388)<RAnZI94>!
C2H5OOH+R9C2H=>CH3CHO+R2OH+C2H2      6.0E11      0.      9.2E3 !
(389)<RAnZI94>!
C2H5OOH+R10C2H3V=>CH3CHO+R2OH+C2H4Z 1.0E12      0.      8.7E3 !
(390)<RAnZI94>!
C2H5OOH+R11C2H5=>CH3CHO+R2OH+C2H6    3.4E11      0.     11.4E3 !
(391)<RAnZI94>!
C2H5OOH+R2OH=>CH3CHO+R2OH+H2O        5.9E12      0.      0.9E3 !
(392)<RAnZI94>!
C2H5OOH+R5CHO=>CH3CHO+R2OH+HCHO      1.8E12      0.     16.7E3 !
(393)<RAnZI94>!
C2H5OOH+R7CH3O=>CH3CHO+R2OH+CH3OH    6.3E11      0.      5.5E3 !
(394)<RAnZI94>!
C2H5OOH+R6CH2OH=>CH3CHO+R2OH+CH3OH   4.2E11      0.     13.6E3 !
(395)<RAnZI94>!
C2H5OOH+R14CH3CO=>2CH3CHO+R2OH       2.0E12      0.     18.5E3 !
(396)<RAnZI94>!
C2H5OOH+R13CH2CHO=>2CH3CHO+R2OH      3.4E11      0.     15.7E3 !
(397)<RAnZI94>!
C2H5OOH+R3OOH=>CH3CHO+R2OH+H2O2      8.0E11      0.     16.2E3 !
(398)<RAnZI94>!
C2H5OOH+R8CH3OO=>CH3CHO+R2OH+CH3OOH 1.1E12      0.     16.7E3 !
(399)<RAnZI94>!
C2H5OOH+R17C2H5OO=>CH3CHO+R2OH+C2H5OOH  1.1E12      0.     16.7E3 !
(400)<RAnZI94>!
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!****** REACTIONS DE R18CH3COOO ****** !
R18CH3COOO+C2H4O#3=CH3COOOH+R13CH2CHO     1.0E12      0.      9.3E3 !
(401,-402)<RAnZI94>!
R18CH3COOO+R3OOH=CH3COOOH+O2              5.5E10      0.     -2.6E3 !
(402,-402)<COX90>!
R18CH3COOO+C2H5OOH=CH3COOOH+R17C2H5OO     5.0E11      0.      9.2E3 !
(403,-403)<RAnZI94>!
R18CH3COOO+C2H5OOH=>CH3CHO+R2OH+CH3COOOH  5.0E11      0.      9.2E3 !
(404)<RAnZI94>!
R18CH3COOO+R18CH3COOO=>2R4CH3+O2+2CO2     1.7E12      0.     -1.0E3 !
(405)<CAVAnAGH90>!

!****** REACTIONS DE CH3COOOH ******!
CH3COOOH=>R4CH3+CO2+R2OH                  1.0E16      0.     40.0E3 !
(406)<CAVAnAGH90>!

!*****************************************************

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!*                                          Primary mechanism of the
oxidation of Ethanol                                          *!
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!*************************************!
!*           REACTIOnS OF ETHANOL      *!
!*************************************!

!Unimolecular initiation

C2H5OH(+M)=R11C2H5+R2OH(+M)       2.95E+22    -2.16        96.6E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /3.80E+88   -19.70       114.5E+3/
                          TROE   /2.094   16539    1.114   161.36/

C2H5OH(+M)=C2H4Z+H2O(+M)          4.90E+9     1.36    65.8E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
                          LOW    /2.404+8    -17.9    84.8E+3/
                          TROE   /2.126     13568   0.969  160.4/

C2H5OH(+M)=R4CH3+R6CH2OH(+M)     6.61E+23  -2.16    88.04E+3
!Tsang, J Chem Kinet 36,436-63,2004!
                         LOW     /1.99E+85  -18.9    104.8E+3/
                         TROE    /2.058     16911    1.071   135.3/
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C2H5OH(+M)=R23C2H4OH+R1H(+M)     2.01E+17    -0.149     101.8E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                          LOW     /4.902E+94   -21.65     123.1E+3/
!Reaction (c5),T=500-1800K
                         !LOW     /2.716E+83   -21.47     38.44E+3/
!Reaction (c5),T=1800-3000K

C2H5OH(+M)=R24C2H4OH+R1H(+M)     7.54E+16    -0.275   94.05E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!
                          LOW     /7.708E+96   -22.47   116.9E+3/
!T=500-1800K
                         !LOW     /5.58E+82    -21.20   37824.5/
!T=1800-3000K
                          DUPLICATE

C2H5OH(+M)=R15C2H5O+R1H(+M)      2.70E+15    0.305    101.3E+3
!T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!
                         LOW      /2.794E+88  -19.76    121.0E+3/
!T=500-1800K;
                        !LOW      /4.246E+91  -23.49    49435.8/
!T=1800-3000K,
                         DUPLICATE

!Bimolecular initiation

C2H5OH+O2=R23C2H4OH+R3OOH           2.100E+13      0.0     52400.0
C2H5OH+O2=R24C2H4OH+R3OOH           1.400E+13      0.0     46300.0
C2H5OH+O2=R15C2H5O+R3OOH            7.000E+12      0.0     55730.0

!Metatheses with abstraction of H-atom

!C2H5OH+R2OH=R23C2H4OH+H2O              6.203E+03      2.68      -576.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R23C2H4OH+H2O               3.60E+06       2.0        950.0
!Nancy, correlation Bozzelli 1999!

!C2H5OH+R2OH=R24C2H4OH+H2O              1.307E+05      2.43     -1456.6
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!
C2H5OH+R2OH=R24C2H4OH+H2O               2.40E+06       2.00     -2100.0
!Nancy, correlation Bozzelli 1999!

C2H5OH+R2OH=R15C2H5O+H2O                2.812E+02      2.97     -580.3
!T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H5OH+B1O=R23C2H4OH+R2OH               9.69E+02       3.23     4658.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007

C2H5OH+B1O=R24C2H4OH+R2OH               1.45E+05       2.47     876.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H5OH+B1O=R15C2H5O+R2OH                1.46E-03       4.73     1727.0
!T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!
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C2H5OH+R1H=R23C2H4OH+H2                 1.88E+03       3.20     7150.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R24C2H4OH+H2                 1.79E+05       2.53     3420.0
!T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H5OH+R1H=R15C2H5O+H2                  5.33E-23       10.58    -4459.0
!T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).
!C2H5OH+R1H=R15C2H5O+H2                 5.36E+4        2.53     8753.6
!T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

!C2H5OH+R4CH3=R23C2H4OH+CH4             6.99E-83      30.14   -15663.0
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R23C2H4OH+CH4              3.30E+02       3.30    12291.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).

!C2H5OH+R4CH3=R24C2H4OH+CH4             1.02E-47      18.51    -9409.4
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R24C2H4OH+CH4              1.99E+01      3.37     7635.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

!C2H5OH+R4CH3=R15C2H5O+CH4              1.01E-51      19.68    -10323.5
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).
C2H5OH+R4CH3=R15C2H5O+CH4               2.035E+0      3.57     7722.0
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)

C2H5OH+R3OOH=R23C2H4OH+H2O2             4.2E+04        2.69     19080
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R24C2H4OH+H2O2             2.80E+04       2.69     15420
!correlation (Dean and Bozzelli 2000)

C2H5OH+R3OOH=R15C2H5O+H2O2           5.400E+04      2.0     15025.0    !
Grana et al.2010

C2H5OH+R11C2H5=R23C2H4OH+C2H6        1.500E+12      0.0     11700.0    !
Konnov 2005!

C2H5OH+R11C2H5=R24C2H4OH+C2H6        4.000E+13      0.0     10000.0    !
Konnov 2005!

C2H5OH+R11C2H5=R15C2H5O+C2H6         2.300E+04      2.0     10525.0    !
Grana et al.2010!

C2H5OH+R6CH2OH=R24C2H4OH+CH3OH       4.000E+11      0.0      9700.0    !
Konnov 2005!

C2H5OH+R7CH3O=R24C2H4OH+CH3OH        2.000E+11      0.0      7000.0    !
Konnov 2005!

C2H5OH+R15C2H5O=C2H5OH+R24C2H4OH     2.000E+11      0.0      7000.0    !
Konnov 2005!
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!*************************************!
!*           REACTIOnS OF R23C2H4OH    *!
!*************************************!

R23C2H4OH=C2H4Z+R2OH                      3.52E-34      11.84   -18737.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                         1.35E+43      -10.29    28035.5
!at 1 atm, T=300-1000K
!                                         7.93E+2        1.51     15180.3
!at 1 Torr, T=300-3000K
!                                         1.51E+33      -6.54     26960.4
!at 100 atm, T=300-1000K
!                                         4.90E-24       9.44    -12183.6
!at 100 atm, T=1000-3000K

R23C2H4OH=R1H+C2H3OH                      3.33E+28      -5.26    35586.9
!at 1 atm,T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!                                         2.67E+15      -1.92    29386.8
!at 1 Torr,T=300-3000K.
!                                         2.67E+27      -4.44    37208.5
!at 100 atm,T=300-3000K

R23C2H4OH=R24C2H4OH                    1.000E+11      0.0     39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81


R23C2H4OH+O2=C2H3OH+R3OOH         1.600E+12      0.0     5000.0

!*************************************!
!*           REACTIOnS OF R24C2H4OH    *!
!*************************************!

R24C2H4OH=CH3CHO+R1H                      8.34E+27       -5.19    35576.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                        8.96E+13       -1.61    28844.3
!at 1 Torr,T=300-3000K
!!                                        5.47E+27       -4.67    37685.4
!at 100 atm,T=300-3000K

R24C2H4OH=R1H+C2H3OH                      2.00E+28      -5.08    39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                        4.44E+21      -3.23    36570.6
!at 1 Torr,T=300-3000K
!!                                        1.22E+30      -5.17    41916.2
!at 100 atm,T=300-3000K

R24C2H4OH=R4CH3+HCHO                      1.14E+22       -3.59   34662.9
!at 1 atm,T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                        5.92E+11       -1.04   28739.0
!at 1 Torr,T=300-3000K
!!                                        4.36E+23       -3.55   38679.0
!at 100 atm,T=300-3000K
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R24C2H4OH+O2=CH3CHO+R3OOH                5.26E+17       -1.637   838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=CH3CHO+R3OOH              5.28E+17       -1.637   839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.

R24C2H4OH+O2=C2H3OH+R3OOH                5.33E+2        2.490    -402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.
!!R24C2H4OH+O2=C2H3OH+R3OOH              7.62E+2        2.446    -296
!at 1 atm, T=300-2000K,Ref: DaSilva et al 2009, JphyschemA, 113,31.

R24C2H4OH+R1H=CH3CHO+H2                  1.361E+09     1.29        2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=R6CH2OH+R4CH3              8.67E+16      -0.891      2903.3
!Rйaction (b2), Lin et al 2011b, JphyschemA,115,3509-22.

R24C2H4OH+R1H=C2H3OH+H2                  4.896E+08      1.70       588.2
!Rйaction (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-
22.

R24C2H4OH+R1H(+M)=C2H5OH(+M)             3.607E+13       0.06      437.2
!Rйaction (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,
                                  LOW /2.767E+56     -15.72
10.7E+03/
                                 Duplicate

R24C2H4OH+R2OH=CH3CHO+H2O             1.500E+13      0.0         0.0
!Konnov 2005

R24C2H4OH+B1O=CH3CHO+R2OH                 9.040E+13      0.0         0.0
!Konnov 2005

!*************************************!
!*           REACTIOnS OF R15C2H5O     *!
!*************************************!

R15C2H5O=R4CH3+HCHO                       4.4E-29      10.69   -16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!                                       1.03E+23    -3.82     19303.7
!at 1 atm, T=300-1000K,
!!                                       2.71E+24    -4.50     21018.7
!at 1 Torr, T=300-1000K,
!!                                       1.87E-28    10.39    -12910.9
!at 1 Torr, T=1000-3000K,
!!                                       5.31E+21    -2.97     19560.1
!at 100 atm, T=300-1000K,
!!                                       9.56E-17    7.66     -7408.3
!at 100 atm, T=1000-3000K,

R15C2H5O=R1H+CH3CHO                       4.25E-32     11.49    -16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!                                       1.33E+38     -8.61    25513.8
!at 1 atm,T=300-1000K
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!!                                        7.25E+31     -7.58    21370.4
!at 1 Torr,T=300-1000K
!!                                        2.14E-34     11.63    -15651.2
!at 1 Torr,T=1000-3000K
!!                                        2.61E+19     -2.15    21996.4
!at 100 atm,T=300-1000K
!!                                        1.64E-27     10.5     -15315.4
!at 100 atm,T=1000-3000K

R15C2H5O+O2=CH3CHO+R3OOH                 6.0E+10       0.0        1.7E+3
!(287,-287)<BAULCH94>!

R15C2H5O+R2OH=CH3CHO+H2O                 1.0E+13       0.0        0.0
!Marinov 1998

R15C2H5O+R1H=CH3CHO+H2                   7.47E+09      1.15       673.7
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22

R15C2H5O+R1H(+M)=C2H5OH(+M)              3.08E+11      0.894      12.9
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22
                                    LOW / 3.772E+51    -15.55
11.1E+3/
                                    DUPLICATE

R15C2H5O+B1O=CH3CHO+R2OH                 1.210E+14     0.0        0.0
!Konnov 2005


!
*************************************************************************
*************************************************!
!
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*************************************************!
!*                                          Secondary mechanism of the
oxidation of Ethanol                                  *!
!
*************************************************************************
*************************************************!
!
*************************************************************************
*************************************************!

!****************************************!
!*           REACTIONS OF C2H3OH        *!
!****************************************!

!C2H3OH+B1O=R13CH2CHO+R2OH                4.4E+10       0.7        3250.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+B1O=R13CH2CHO+R2OH                1.4E+13       0.0        2.3E3
!Acйtaldйhyde! (219,-219)<CAVAnAGH90>
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!C2H3OH+R1H=R13CH2CHO+H2              2.700E+04     2.5
-1900.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R1H=R13CH2CHO+H2              1477.2        3.077
7230       !T=300-3000!RAO 2011! J Phys Chem 2011,115
!                                    REV   /1.41         3.721     24600/
C2H3OH+R1H=R13CH2CHO+H2                 1.31E+5       2.58      1220.0
!Acйtaldйhyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem
A,114,755-764.

!C2H3OH+R2OH=R13CH2CHO+H2O            1.500E+06     2.0
-1520.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R2OH=R13CH2CHO+H2O               2.300E+10     0.73     -1100.0
!Acйtaldйhyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2          3.200E+03     2.6
12400.0    !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
!C2H3OH+R3OOH=R13CH2CHO+H2O2          1.626E+12     0.0
16295.1    !Syn_CH2H3OH! ajoutй le 20/10/2011 !Altarawneh et al 2011!
T=700-1300K!
C2H3OH+R3OOH=R13CH2CHO+H2O2             1.0E12        0.0       10.0E3
!Acйtaldйhyde!(311,-311)<CAVAnAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4           5.000E+10     0.0
7300.0     !<PAG,Ulisier paras. des mйtathиses d'atome H allylique
secondaire>!
C2H3OH+R4CH3=R13CH2CHO+CH4              2.0E-6        5.6       2.5E+3
!Acйtaldйhyde! (216,-216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6             0.740         3.5       4140.0
!<PAG,Ulisier paras. des mйtathиses d'atome H allylique secondaire>!
C2H3OH+R11C2H5=R13CH2CHO+C2H6           1.3E12        0.0       8.5E3
!Acйtaldйhyde! (218,-218)<HOHLEIn70>

C2H3OH=CH3CHO                           4.5E+06       1.8       5.1E+4
!Prof. Fournet
!!C2H3OH=CH3CHO                         8.590E+11     0.318     55900.00
! DaSilva 2006!
  !!                                REV/   1.050E+09     1.202
66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH              1.49E+05      1.67      6810.0
!P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29
C2H3OH+R1H=CH3CHO+R1H                   1.00E+13      0.00      1506.0
!T=300-2000K!form observation in Huynh et al 2009, j phys chem A
113,3177-3185:

!"The rate of this reaction is close to that of the H addition to C2H4:
C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+CO2+H2                1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5
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!C2H3OH+R2OH=HCHO+R6CH2OH                1.40E+12     0.00      -1040.0
!Nancy, tableau A-I-5

!C2H4+OH<=>C2H3OH+H                      1.070E+04    2.600     4133.00
!Senosiain et al 2006
C2H4Z+R2OH=C2H3OH+R1H                    4.000E+12    0.000     4880.00
!Hippler et al 2000

!*************************************!
!*           REACTIOnS OF CH3CHO       *!
!*************************************!

CH3CHO+R2OH=R14CH3CO+H2O                 2.300E+10   0.73
-1100.0     ! Konnov 2005!
CH3CHO+R1H=H2+R14CH3CO                   1.31E+5     2.58
1220.0      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
CH3CHO+R4CH3=R14CH3CO+CH4                2.0E-6      5.6
2.5E+3      !(216,-216)<BAULCH94>! T=300-1250K
CH3CHO+B1O=R14CH3CO+R2OH                 1.4E+13     0.
2.3E3       !(219,-219)<CAVAnAGH90>!
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO           8.1E10      0.
3.7E3       !(217,-217)<SCHERZER87>T=480-520K!NIST
CH3CHO+R11C2H5=C2H6+R14CH3CO             1.3E12      0.
8.5E3       !(218,-218)<HOHLEIn70>!
CH3CHO+R7CH3O=R14CH3CO+CH3OH             5.000E+12   0.0
0.0         !Konnov 2005!
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO         3.000E+12   0.0
11200.0     !Konnov 2005!

!CH3CHO+R2OH=R13CH2CHO+H2O               1.600E+13   0.0
2000.0      !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J
Chem Kin 2008,40,73-102
CH3CHO+R2OH=R13CH2CHO+H2O                3.370e+11   0.0
-619.98     !Mech Sandiego=ref:Juan Li's PhD thesis!
!CH3CHO+R1H=R13CH2CHO+H2                 4.40E+14    0.0
10.0E+3     !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R1H=R13CH2CHO+H2                  2.72E+03    3.1
5206.5      !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-
764.
!CH3CHO+R4CH3=R13CH2CHO+CH4              6.00E+12    0.0
11000.0     !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm
CH3CHO+R4CH3=R13CH2CHO+CH4               2.45E+1     3.15
5727.0      !Marinov 1998
CH3CHO+B1O=R13CH2CHO+R2OH                3.720E+13   -0.2
3556.0      !Marinov 1998




!****** REACTIONS DE C2H5 ******!
R11C2H5+R10C2H3V=>C4H8Y                    1.5E13      0.         0. !
(61,-61)<TSAnG86>!
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!R11C2H5+R11C2H5=>C4H10                    1.1E13      0.          0. !
(65,-65)<BAULCH94>!


!****** REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE ******!

C2H3CHO+R2OH=CH2CHCO+H2O                   1.0E13      0.0    0.0    !
<MARInOV>!
C2H3CHO+B1O=CH2CHCO+R2OH                   7.2E12      0.0    2.0E3  !
<MARInOV>!
C2H3CHO+B1O=CH2COZ+R5CHO+R1H               5.0E7       1.76   0.08E3 !
<MARInOV>!
C2H3CHO+R1H=CH2CHCO+H2                     4.0E13      0.0    4.2E3  !
<MARInOV>!
C2H3CHO+R1H=C2H4Z+R5CHO                    2.0E13      0.0    3.5E3  !
<MARInOV>!
C2H3CHO+O2=CH2CHCO+R3OOH                   3.0E13      0.0   38.5E3  !
<MARInOV99>+ MF correlation Baptiste
CH2CHCO=R10C2H3V+B2CO                      1.0E14      0.0   34.0E3  !
<MARInOV>!
CH2CHCO+B1O=R10C2H3V+CO2                   1.0E14      0.0    0.0    !
<MARInOV>!
C3H5Y+R3OOH=>C2H3CHO+R1H+R2OH               7.0E18     -2.0    0.0    !
<TSAnG91>!
C3H5Y+O2=C2H3CHO+R2OH                      1.8E13     -0.41   22.9E3 !
<BOZELLI93>!
C3H5Y+B1O=C2H3CHO+R1H                      1.8E14      0.0     0.0   !
<SLAGLE92>!

!*****************************************************!
!       REACTIONS DES ESPECES NON OXYGEnNS EN C3      !
!*****************************************************!

!****** REACTIONS DE C3H2  ***** (CHCCH(..))*****!

B4CH+C2H2=C3H2+R1H                         2.1E14       0.0        -0.5E3 !
<MILLER92/BAULCH94>!
C3H2+B1O=R9C2H+R1H+B2CO                    3.0E13       0.0         0.0   !
<PEETERS97>!
C3H2+R2OH=C2H2+R5CHO                       5.0E13       0.0         0.0   !
<MILLER92>!
C3H2+O2=R12CHCOZ+B2CO+R1H                  5.0E13       0.0         0.0   !
<MILLER92>!


!****** REACTIONS DE C3H3 ***** (CHCCH2(.)) Propargyl*****stablilise par
resonnance !

B6CH2+C2H2=C3H3+R1H                      1.8E14       0.0         0.0   !
<MILLER87/BAULCH94>!
C3H3+R1H=C3H2+H2                         2.0E13       0.0         0.0   !
<MILLER92/BRAUn89>!
C3H3+B1O=R9C2H+HCHO                      1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
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C3H3+R2OH=C3H2+H2O                      2.0E13       0.0          0.0   !
<MILLER92>!
C3H3+R2OH=R10C2H3V+R5CHO                4.0E13       0.0          0.0   !
<WAnG97>!
C2H2+R12CHCOZ=C3H3+B2CO                 1.0E11       0.0          3.0E3 !
<MILLER92>!
C3H3+O2=CH2COZ+R5CHO                    3.0E10       0.0          2.9E3 !
<MILLER92/SLAGUE88>!
C3H2+R1H=C3H3                           1.0E14       0.0          0.0   !
<est>!
C3H3+R3OOH=>R2OH+R9C2H+HCHO              1.0E15      -0.8          0.0   !
<Heyberger>!
C3H3+C3H3=C6H6#                         1.0E12       0.0          0.0   !
<STEIn90>shocktube!
C3H3+C3H3=C6H5#+R1H                      1.0E12       0.0          0.0   !
<STEIn90>flame!



!****** REACTIONS DE pC3H4 ***** (CH3CCH) Propyne *****!

!pC3H4=>aC3H4                            2.1E12       0.0         60.0E3
     !<HIDAKA89>!
pC3H4+M=C3H3+R1H+M                       4.7E18       0.0         80.0E3
     !<HIDAKA89>!
C2H2+B5CH2=pC3H4                         3.5E12       0.0          0.0
     !<TSAnG86>!

pC3H4=R9C2H+R4CH3                        4.2E15       0.0        125.0E3  !
<KInGAS1500>!
pC3H4+O2=C3H3+R3OOH                      2.1E12       0.0         40.8E3  !
<est Ingham>!
pC3H4+R1H=C2H2+R4CH3                     1.3E5        2.5         1.00E3  !
<hidaka89> !
pC3H4+R1H(+M)=tC3H5(+M)                  8.5E12       0.0          1.7E3  !
<WAGnER72>!
                    LOW   /5.6E25     -7.27     6.58E3/
          !<Marinov97!
pC3H4+R1H(+M)=sC3H5(+M)                  5.8E12       0.0          3.1E3  !
     <WAGnER72>!
                    LOW   /3.8E25     -7.27     7.98E3/
          !<estimated>!
pC3H4+R4CH3=C3H3+CH4                     2.2E0        3.5          5.7E3  !
<asTSAnG91>!
pC3H4+R1H=C3H3+H2                        1.7E5        2.5          2.5E3  !
<asTSAnG91>

pC3H4+R9C2H=C3H3+C2H2                    3.6E12       0.0            0.0
     !<asTSAnG91>!
pC3H4+R10C2H3V=C3H3+C2H4Z                2.2E0        3.5          4.7E3  !
<asTSAnG91>!
pC3H4+R11C2H5=C3H3+C2H6                  2.2E0        3.5          6.6E3  !
<asTSAnG91>!
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pC3H4+B1O=R12CHCOZ+R4CH3                1.5E13      0.0         2.1E3  !
<WARnATZ84>!
pC3H4+B1O=R2OH+C3H3                     3.4E4       2.16        4.8E3  !
<<ADUSEI, G.Y, 1996>!
pC3H4+R2OH=CH2COZ+R4CH3                 4.3E11      0.0        -0.8E3  !
<BOODAGHIAnS87>!
pC3H4+R2OH=R1H+C2H3CHO                  4.3E11      0.0        -0.8E3  !
<asBOODAGHIAnS87>!
pC3H4+R2OH=C3H3+H2O                     3.1E6       2.0        -0.3E3  !
<asTSAnG91>!
pC3H4+R3OOH=C2H4Z+B2CO+R2OH             6.0E9       0.0         8.0E3  !
as296<TSAnG86>!
pC3H4+R3OOH=C3H3+H2O2                   9.6E3       2.6        13.9E3  !
<asTSAnG91>!
pC3H4+R7CH3O=CH3OH+C3H3                 2.0E12      0.0         4.0E3  !
<Heyberger>!


!******** REACTIONS DE aC3H4 ***** (CH2CCH2) Allene  *******!

aC3H4=pC3H4                             2.5E12      0.0        59.0E3  !
<HIDAKA89>!
aC3H4+M=C3H3+R1H+M                      2.0E18      0.0        80.0E3  !
<HIDAKA89>!
aC3H4+O2=C3H3+R3OOH                     2.8E13      0.0        39.0E3  !
<Estimation Ingham>!
aC3H4+R1H(+M)=C3H5Y(+M)                       4.0E12      0.0
2.7E3      !<WAGnER72>!
                    LOW   /5.6E33       -5.0   4.44E3/
           !<Marinov97> !
aC3H4+R1H(+M)=tC3H5(+M)                 8.5E12      0.0         2.0E3  !
<WAGnER72>!
                    LOW   /1.1E34     -5.0     4.44E3/
           !<Marinov97!
C2H4Z+B4CH=aC3H4+R1H                    1.3E14      0.0        -0.3E3  !
<BAULCH94base>!
R10C2H3V+B5CH2=aC3H4+R1H                3.0E13      0.0         0.0    !
<MILLER92>!
iC4H3+B5CH2=aC3H4+R9C2H                 2.0E13      0.0         0.0    !
<MILLER92>!
aC3H4+B1O=R1H+B2CO+R10C2H3V             6.6E12      0.0         3.0E3  !
<Aleksandrev nist>!
aC3H4+R2OH=CH2COZ+R4CH3                 2.0E12      0.0        -0.2E3  !
<LIU88>!
aC3H4+R2OH=HCHO+R10C2H3V                2.0E12      0.0        -0.2E3  !
<LIU88>!

aC3H4+R1H=C3H3+H2                       1.3E6       2.53        9.2E3  !
<est.butatiene>!
aC3H4+B1O=C3H3+R2OH                     6.2E12      0.0         1.9E3  !
<fromAleksandrev nist>!
!d'aprиs leur vitesse de rйaction total et d'addition !
aC3H4+R2OH=C3H3+H2O                     6.2E6       2.0         0.4E3  !
<est.butadiene>!
```

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aC3H4+R4CH3=C3H3+CH4                    2.0E12      0.0         7.7E3  !
<WU87>!
aC3H4+R9C2H=C3H3+C2H2                   1.0E13      0.0         0.0    !
<WU87>!
aC3H4+C3H5Y=C3H3+C3H6Y                  2.0E12      0.0         7.7E3  !
<DAGAUT92>
aC3H4+R7CH3O=CH3OH+C3H3                        4.0E12      0.0
9.6E3      !<correlations a partir de Heyberger>!
aC3H4+R11C2H5=C2H6+C3H3                   5.0E14      0.0        19.8E3
      !<asbutadiene>!
aC3H4+R10C2H3V=C2H4Z+C3H3             5.0E14      0.0        19.8E3   !
<asbutadiene>!
!aC3H4+R4CH3=C4H7T                      5.7E10      0.0         6.8E3  !
<Scherzer>!
!aC3H4+R4CH3=C4H7T                      3.4E11      0.0         7.4E3
      !<Tsang91x2>!
!aC3H4+R4CH3=iC4H7                      1.6E11      0.0         5.0E3
      !<Tsang73>!
!aC3H4+R4CH3=C4H7T                           0.8E11      0.0
7.4E3      !<Tsang91x2/4>!
aC3H4+R4CH3=iC4H7                       0.4E11      0.0         5.0E3
      !<Tsang73/3>!


!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K
(Tsang91)!
!aC3H4+C3H3=C6H6#+R1H                  1.4E12       0.0        10.0E3  !
<HIDAKA89>!


!******** REACTIONS DE cC3H4 ***** cyclopropene *********!

cC3H4=aC3H4                             1.5E14      0.0    50.5E3  !
<Karni>
cC3H4=pC3H4                             7.1E13      0.0    47.8E3  !
<Karni>
cC3H4+R1H=cC3H3+H2                      5.4E4       2.5    -1.9E3  !
<Heyberger>!
cC3H4+R2OH=cC3H3+H2O                    3.0E6       2.0    -1.5E3  !
<Heyberger>!
cC3H4+R2OH=C2H4Z+R5CHO                  2.8E12      0.0    -1.0E3  !
<Heyberger>!
cC3H3+R3OOH=R2OH+C2H2+R5CHO             1.0E15     -0.8     0.0    !
<Heyberger>!
cC3H3+R4CH3=cC4H6                       1.0E13      0.0     0.0    !
<estimation>!
cC3H3+R1H=cC3H4                         1.0E14      0.0     0.0    !
<estimation>!

!****** REACTIONS DE C3H5Y ***** (CH2CHCH2(.)) Allyl *****stablilise par
resonnance !

!C3H5Y+R1H=C3H6Y                        2.0E13      0.0         0.0  !
<TSAnG91>!
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C3H5Y+R1H=aC3H4+H2                      1.8E13      0.0         0.0  !
TSANG 91!*
C3H5Y+R1H=C3H6Y                         1.0E14      0.0         0.0  !
<allara>!!


!rйaction importante pour la formation de propиne!
C3H5Y+R4CH3=aC3H4+CH4                   3.0E12     -0.32     -0.1E3    !
<TSAnG91>!
C3H5Y+R4CH3=C4H8Y                       1.0E14     -0.32     -0.1E3    !
<TSAnG91>!
C3H5Y+R2OH=aC3H4+H2O                    6.03E12     0.0         0.0  !
Tsang 91!
!peu d'effet de fall off!
C3H5Y+R10C2H3V=aC3H4+C2H4Z              2.4E12      0.0         0.0  !
<TSAnG91>!
!C3H5Y+R11C2H5=aC3H4+C2H6               9.6E11      0.0      -0.1E3    !
<TSAnG91>!
C3H5Y+R11C2H5=aC3H4+C2H6                2.0E13      0.0      -0.1E3    !
<TSAnG91>MODIF!!!!!
C3H5Y+B1O=R10C2H3V+HCHO                 1.8E14      0.0         0.0  !
<SLAGLE90,LEUnG95>!
!processus non elementaire impliquant la formation-decomposition de
l'hydroperoxyde
!C3H5Y+C3H3=C6H6#+2R1H                  5.6E20     -2.535     1.7E3    !
<MARInOV97>!
C3H5Y+C3H5Y=aC3H4+C3H6Y                 8.4E10      0.0      -0.3E3    !
<TSAnG91>!


!****** REACTIONS DE sC3H5 ***** (CH3CHCH(.)) 2-methyl vinyl *****!

sC3H5=C3H5Y                            5.0E13      0.0        37.0E3 !
<WEISSMAn89>!
R4CH3+C2H2=sC3H5                       6.0E11      0.0       7.7E3 !
<BAULCH94>!

!****** REACTIONS DE tC3H5 ***** (CH3C(.)CH2) 1-methyl vinyl *****!

tC3H5+R1H=aC3H4+H2                      3.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5+R4CH3=aC3H4+CH4                   1.0E11      0.0         0.0   !
<DAGAUT90>!
tC3H5+R10C2H3V=aC3H4+C2H4Z              1.0E12      0.0         0.0   !
<LEUnG95>!
tC3H5+R11C2H5=aC3H4+C2H6                1.0E12      0.0         0.0   !
<LEUnG95>!
tC3H5+B1O=CH2COZ+R4CH3                  1.8E14      0.0         0.0   !
<LEUnG95>!
tC3H5+O2=R4CH3+B2CO+HCHO                4.3E12      0.0         0.0   !
<DAGAUT90>!
tC3H5=C3H5Y                             2.0E13      0.0        47.0E3 !
<Weissman89>!
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!****** REACTIONS DE C3H6Y ***** (CH3CHCH2) propene *****!

C2H4Z+B6CH2=C3H6Y                       9.6E13      0.0        0.0  !
<BAULCH94>!
C2H4Z+B5CH2=C3H6Y                       3.2E12      0.0      5.1E3  !
<BAULCH94>!
!duplicate R10C2H3V+R4CH3=C3H6Y         2.5E13      0.0        0.0  !
<TSAnG86>!
C2H4Z+R4CH3=C3H6Y+R1H                   6.6E11      0.0     15.9E3  !
<TSAnG86>!
R11C2H5+B6CH2=C3H6Y+R1H                 9.0E12      0.0        0.0  !
<TSAnG86>!
C2H6+B4CH=C3H6Y+R1H                     1.1E14      0.0     -0.3E3  !
<BAULCH94>!
C3H6Y+R1H=sC3H5+H2                      7.83E5      2.5    12.28E3  !
<TSAnG92>!
C3H6Y+R1H=tC3H5+H2                      3.9E5       2.5     5.82E3  !
<TSAnG92>!
C3H6Y+R1H=C3H5Y+H2                      1.7E5       2.5      2.5E3  !
<TSAnG91>!
C3H6Y+R4CH3=C3H5Y+CH4                   2.2E0       3.5      5.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=sC3H5+CH4                   8.4E-1      3.5     11.7E3  !
<TSAnG91>!
C3H6Y+R4CH3=tC3H5+CH4                   1.3E0       3.5     12.9E3  !
<TSAnG91>!
C3H6Y+R11C2H5=C3H5Y+C2H6                2.2E0       3.5      6.6E3  !
<TSAnG91>!
!C3H6Y+B1O=>CH2COZ+R1H+R4CH3             1.2E+5      2.56   -1130.0  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+B1O=C3H5Y+R2OH                    1.7E11      0.7      5.9E3  !
<TSAnG91>!
!C3H6Y+R2OH=HCHO+R11C2H5                 1.45E12     0.0     -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
!C3H6Y+R2OH=R4CH3+CH3CHO                1.45E12     0.0     -0.9E3  !
<TSAnG91>! MF!!ds мйca PRF
C3H6Y+R2OH=C3H5Y+H2O                    3.1E6       2.0     -0.3E3  !
<TSAnG91>!
C3H6Y+R2OH=sC3H5+H2O                    1.1E6       2.0     1.45E3  !
<TSAnG91>!
C3H6Y+R2OH=tC3H5+H2O                    2.1E6       2.0      2.8E3  !
<TSAnG91>!
C3H6Y+O2=C3H5Y+R3OOH                    1.9E12      0.0     39.0E3  !
<WALKER93>!
C3H6Y+R3OOH=C3H5Y+H2O2                  9.6E3       2.6     13.9E3  !
<TSAnG91>!

C3H6Y+R9C2H=pC3H4+R10C2H3V             1.2E13       0.0     0.0     !TSANG
91 mehdi!

!****** REACTIONS DE cC3H6 ***** cyclopropane *****!
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cC3H6=C3H6Y                          4.6E14      0.0    62.6E3  !
<Hidaka87>!
cC3H6+R1H=C3H5Y+H2                    1.6E14      0.0   11.7E3   !
<Marshall86>!
cC3H6+R2OH=C3H5Y+H2O                       7.0E7       1.5    1.0E3   !
<Dobe82>!
cC3H6+R4CH3=C3H5Y+CH4                    2.0E11      0.0    9.6E3   !
<Exgas>!

!****** REACTIONS DE R19C3H7 et iC3H7 ***** CH3CH2CH2(.) et  CH3CH(.)CH3
***** !

!R19C3H7 = R4CH3+C2H4Z                       6.400E+12   0.00    31000.0!!
ds мйса PRF
!R19C3H7 = R1H+C3H6Y                         3.000E+13   0.00   38000.00!!
ds мйса PRF
iC3H7 = R1H+C3H6Y                          6.000E+13   0.00   39000.00
R19C3H7 = iC3H7                              1.960E+10   1.00   38600.00
!R19C3H7+O2 =R3OOH+C3H6Y                      1.600E+12   0.00    5000.00
R19C3H7+O2 =R3OOH+C3H6Y                      3.7e16   -1.63    3420 !
2003DES/KLI4415-4427
iC3H7+O2 = R3OOH+C3H6Y                     1.400E+12   0.00    5000.00

!****** Propane (C3H8) chemistry ******!

R11C2H5+R4CH3=C3H8         3.4E13      0.          0.  !(59,-
59)<BAULCH94>!
C3H8+O2=>R3OOH+iC3H7        1.4E+0013  0.000  50323.7  ! BI 2 CN
C3H8+O2=>R3OOH+R19C3H7        4.2E+0013  0.000  53033.0  ! BI 3 CN
B1O+C3H8=>R2OH+iC3H7        2.6E+0013  0.000   5200.0  ! ME 15 CW
B1O+C3H8=>R2OH+R19C3H7        1.0E+0014  0.000   7850.0  ! ME 16 CW
C3H8+R1H=>H2+iC3H7          9.0E+0006  2.000   5000.0  ! ME 17 CW
!C3H8+R1H=>H2+R19C3H7          5.7E+0007  2.000   7700.0  ! ME 18 CW!!ds
мйса PRF
C3H8+R2OH=>H2O+iC3H7       2.6E+0006  2.000   -765.0  ! ME 19 CW
!C3H8+R2OH=>H2O+R19C3H7         5.4E+0006  2.000    450.0  ! ME 20 CW!!ds
мйса PRF
C3H8+R3OOH=>H2O2+iC3H7     4.0E+0011  0.000  15500.0  ! ME 21 CN
!C3H8+R3OOH=>H2O2+R19C3H7       1.2E+0012  0.000  17000.0  ! ME 22 CN!!ds
мйса PRF
C3H8+R4CH3=>CH4+iC3H7      2.0E+0011  0.000   9600.0  ! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7        6.0E-0001  4.000   8200.0  ! ME 24 CN!!ds
мйса PRF
C3H8+R5CHO=>HCHO+iC3H7     1.0E+0007  1.900  17000.0  ! ME 25 CN
C3H8+R5CHO=>HCHO+R19C3H7        2.0E+0005  2.500  18500.0  ! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7    2.0E+0011  0.000  11000.0  ! ME 33 CN
!C3H8+R11C2H5=>C2H6+R19C3H7    6.0E+0011  0.000  13500.0  ! ME 34 CR!!ds
мйса PRF
C3H8+iC3H7=>C3H8+R19C3H7        8.4E-0003  4.200   8700.0  ! ME 35 CN
R1H+iC3H7=>C3H8             8.3E+0012  0.000      0.0  ! CO 36 K

!****************Reactions of Acetone**************************!
!R14CH3CO+R4CH3=>C2H6CO                     4.0E15     -0.8        0. !
(231,-231)<TSAnG86>!
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R14CH3CO+R4CH3=>C2H6CO                    2.7E15     -0.8        0. !
(231,-231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low
pressure.
iC3H7+B1O=>C2H6CO+R1H                  1.0          0.0         0.0     !
Tsang88 (Nist)
C2H6CO+O2=>R3OOH+CH2COZ+R4CH3          4.2E12       0.0         49.28E3 !
Kingas!
C2H6CO+B1O=>CH2COZ+R4CH3+R2OH          1.02E14      0.0         7.85E3  !
Buda!
C2H6CO+R1H=>CH2COZ+R4CH3+H2            5.70E07      2.0         7.70E3

C2H6CO+R2OH=>CH2COZ+R4CH3+H2O          5.34E06      2.0         0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4         6.00E-1      4.0         8.20E3

C2H6CO+R3OOH=>CH2COZ+R4CH3+H2O2        1.20E12      0.0         17.0E3

!*****************Reactions of Propanal************************!

!R5CHO+R11C2H5=>C2H5CHO                    1.8E13       0.          0.
!(141,-141)<TSAnG86>!
!C2H5CHO=R5CHO+R11C2H5                     1.07E+14     0.0       62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240
R5CHO+R11C2H5=C2H5CHO                     3.4E+13      0.0       0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R5CHO+R11C2H5                     2.45E+15     0.0       72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)
R13CH2CHO+R4CH3=C2H5CHO                  3.4E+13      0.0       0.0
!= "CH3+C2H5=C3H8".
!C2H5CHO=R13CH2CHO+R4CH3                 1.000e+17   0.0   8.465e+04   !
asC4H10 Dean, J.Phys.Chem. 89 (1985) 4600-4608
!C2H5CHO=R4CH3+R13CH2CHO                  7.00E+15     0          81703
!Baulch et al 1992,J. Phys.Chem.Ref.Data 21 411–429.
B1O+C3H6Y=>C2H5CHO                        1.000E+12    0          5000.0
!Mech Franssoldati
!C2H5CHO+R1H=H2+B2CO+R11C2H5               4.0E13       0.0        4.2E3
!<Heyberger>! ADZ 714
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5             4.0E12       0.0        0.5E3
!<Heyberger>! ADZ 715

!C2H5CHO=R4CH3+R13CH2CHO                  2.00E+16     0          83800.
!Mech Franssoldati
C2H5CHO+R1H=H2+R25C2H5CO                  1.17E+11     0.0        6000
!Decottignies et al.2002.
!C2H5CHO+R1H=R25C2H5CO+H2                 1.200E+14   0.00     7000.0   !
Yasunaga et
C2H5CHO+B1O=R2OH+R25C2H5CO                5.000e+12    0.0
1.790e+03  !Curran et al. Fuel (2011) 90(1) 331–338.
C2H5CHO+R2OH=H2O+R25C2H5CO                2.690e+10    0.760
-3.400e+02  !Curran et al. Fuel (2011) 90(1) 331–338.
!C2H5CHO+R2OH=R25C2H5CO+H2O               2.650E+12   0.00     -730.0   !
Atkinson et
R25C2H5CO=B2CO+R11C2H5                    2.95E+12     0.0       11100.0
!Decottignies et al.2002.
```

```
!R25C2H5CO=>R11C2H5+B2CO                    1.834e+15  -0.73  1.291e+04
!Glaude et a
!*************************************************

!*************************************************


!*************************************************!
!     REACTIONS DES ESPECES NON OXYGENES EN C4     !
!*************************************************!

!****** REACTIONS DE C4H2  ***** (CH///CC///CH) diacetylene ***** !

R9C2H+R9C2H=C4H2                      1.8E13       0.0         0.0   !
<TSAnG86>!
2C2H2=C4H2+H2                         1.5E13       0.0      42.7E3     !
<LEUnG95>!
C2H2+R9C2H=C4H2+R1H                   9.0E13       0.0         0.0   !
BAULCH94!
!C4H2+R1H=C2H2+R9C2H                  6.0E14       0.0      15.4E3     !
<MEREDITH86>!
C4H2+R2OH=>R5CHO+C3H2                  6.7E12       0.0      -0.4E3    !
<LEEDS-website>!
C4H2+O2=R12CHCOZ+R12CHCOZ             9.6E12       0.0      31.1E3     !
<HIDAKA02>!!!
C4H2+R9C2H=>C6H2+R1H                  4.0E13       0.0         0.0   !
<MEREDITH86>!
C6H2+R1H=>C4H2+R9C2H                  9.3E14       0.0      15.1E3     !
<MEREDITH86>!

!****** REACTIONS DE nC4H3  ***** (ĽCH//CHC///CH) **********!

nC4H3(+M)=C4H2+R1H(+M)                1.0E14       0.0      36.0E3     !
<MILLER92>!
          LOW   /1.0E14 0.0 30E3/
          TROE / 1.0  1.0  1.0E8/
C3H3+B4CH=nC4H3+R1H                   7.0E13       0.0         0.0   !
<MILLER92>!
!C3H3+B4CH=nC4H3+R1H                  5.0E13       0.0         0.0   !
<MILLER92>!
R9C2H+R10C2H3V=nC4H3+R1H              1.8E13       0.0         0.0   !
<TSAnG86>!
nC4H3+R1H=iC4H3+R1H                   2.4E11       0.79     2.41E3     !
<WAnG97>20Torr!
nC4H3+R1H=C4H2+H2                     0.6E13       0.0         0.0   !
<0.5*la cst de la react(c2h3+h)>!
2C2H2=nC4H3+R1H                       1.0E12       0.0      64.1E3   !
<LEUnG95>!
nC4H3+R2OH=C4H2+H2O                   1.5E13       0.0         0.0   !
<0.5* la cst de la react(c2h3+oh)>!
!***
!nC4H3+C2H2=C6H4#+R1H                  1.64E9       0.73     12.2E3   !
<WESTMORELAnD89, p=2.6kPa>!
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nC4H3+C2H2=C6H4#+R1H                3.0E-11      6.48      6.6E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H4+R1H                 29.6         3.33      9.6E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H4+R1H                2.77E-7      5.59      6.0E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=lC6H5                     1.73E11     -0.41      4.0E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=lC6H5                    6.17E15     -1.51      4.8E3      !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H3+C2H2=C6H5#                     3.33E24     -3.89      9.2E3    !
<WESTMORELAnD89, p=2.6kPa>!
nC4H3+C2H2=C6H5#                    7.0E14      -0.86      6.4E3      !
<WESTMORELAnD89, p=101kPa>!
!***


!****** REACTIONS DE iC4H3  ***** (CH2//CĽC///CH) *****

iC4H3=nC4H3                          1.5E13       0.0      67.8E3   !
<LEUnG95>!
iC4H3(+M)=C4H2+R1H(+M)               1.0E14       0.0      55.0E3     !
<MILLER92>!
           LOW  /2.0E15 0.0 48E3/
           TROE /1.0  1.0  1.0E8/
C3H2+B5CH2=iC4H3+R1H                 1.2E14       0.0       0.8E3     !
as(7)<BAULCH94>!
iC4H3+R1H=2C2H2                      2.40E19      -1.6       2800   !
<WAnG97>20Torr! !
C3H3+B4CH=iC4H3+R1H                  7.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R1H=C4H2+H2                    1.2E13       0.0         0.0   !
<equiv a la cst de la react(c2h3+h)>!
iC4H3+B1O=CH2COZ+R9C2H               2.0E13       0.0         0.0   !
<MILLER92>!
iC4H3+R2OH=C4H2+H2O                  3.0E13       0.0         0.0   !<
equiv a la cst de la react(c2h3+oh)>!
iC4H3+O2=CH2COZ+R12CHCOZ             1.0E12       0.0         0.0   !
<MILLER92>!
*
iC4H3+R10C2H3V=2C3H3                 4.0E12       0.0         0.0   !
MILLER 92 !
iC4H3+R10C2H3V=>lC6H5+R1H             6.0E12       0.0         0.0   !
MILLER 92!

!****** REACTIONS DE C4H4  ***** (CH2//CHC///CH) vinylacetylene *****!

C3H3+B5CH2=C4H4+R1H                  4.0E13       0.0           0.0 !
<MILLER92>!
R10C2H3V+C2H2=>C4H4+R1H              2.0E13       0.0        25.1E3 !
(40,-40)<DOUTE95>!
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C4H4+R1H=>R10C2H3V+C2H2                 2.0E13       0.0        12.4E3 !
<DOUTE95>
C2H4Z+R9C2H=C4H4+R1H                    1.2E13       0.0           0.0 !
(50,-50)<TSAnG86>!
C4H4+R1H=nC4H3+H2                       2.0E7        2.0         15.E3 !
<Miller 92>!
C4H4+R1H=iC4H3+H2                       3.0E7        2.0          5.E3 !
<Miller 92>!
R9C2H+C4H4=>C2H2+iC4H3                  4.0E13       0.0           0.0 !
<MEREDITH86>!
C2H2+iC4H3=>R9C2H+C4H4                  3.0E13       0.0        27.9E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+nC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
nC4H3+C2H4Z=>R10C2H3V+C4H4              3.5E11       0.0        13.4E3 !
<MEREDITH86>!
R10C2H3V+C4H4=>C2H4Z+iC4H3              5.0E11       0.0        16.3E3 !
<MEREDITH86>!
iC4H3+C2H4Z=>R10C2H3V+C4H4              1.3E11       0.0        24.1E3 !
<MEREDITH86>!
C4H4+C2H2=C6H5#+R1H                     1.0E09       0.0       30.02E3 !
BENSON  !MF
C4H4+R10C2H3V=C6H6#+R1H                 1.9E12       0.0         2.5E3 !
<LInSTEDT96>!
C4H4+B1O=aC3H4+B2CO                     3.0E13       0.0         1.8E3 !
<LEUnG95>!
C4H4+B1O=pC3H4+B2CO                     2.7E13       0.0         1.8E3 !
<MILLER>!
C4H4+R2OH=nC4H3+H2O                     7.5E6        2.0         5.0E3 !
<MILLER92>!
C4H4+R2OH=iC4H3+H2O                     1.0E7        2.0         2.0E3 !
<MILLER92>!
aC3H4+aC3H4=C2H4Z+C4H4                  1.0E15       0.0        48.0E3 !
<HIDAKA89>!


!****** REACTIONS DE tC4H4  ***** (CH2//C//C//CH2) *****!

tC4H4+R2OH=iC4H3+H2O                    2.0E7        2.0         2.0E3   !
<Marinov>!
tC4H4+R1H=iC4H3+H2                      3.0E7        2.0         6.0E3   !
<Marinov>!

!****** REACTIONS DE nC4H5  ***** (ĽCH//CHCH//CH2) *****

nC4H5(+M)=R1H+C4H4(+M)                  1.0E14       0.0       37.0E3      !
<MILLER92>!
            LOW   /1.00e+14 0.0 30000/
nC4H5+R1H=C4H4+H2                       1.5E13       0.0           0.0    !
<WAnG97>!
nC4H5+R1H=iC4H5+R1H                     1.0E14       0.0           0.0    !
<MILLER92>!
nC4H5+R4CH3=C5H8                        1.0E13       0.0           0.0    !
<estimated> !
```

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nC4H5=C2H2+R10C2H3V                    1.0E14       0.0       43.9E3      !
<HIDAKA96>!
!***
!MF car lC6H6 n'intervient qu'ici
!nC4H5+C2H2=lC6H6+R1H                   1.17E-15     7.84       2.0E3  !
<WESTMORELAnD89, p=2.6kPa>!
!nC4H5+C2H2=lC6H6+R1H                  3.47E-15     7.73       2.5E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H6#+R1H                   1.90E7       1.47       4.2E3  !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H6#+R1H                  2.38E8       1.18       3.7E3  !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=lC6H7                       8.74E12     -1.27       3.6E3 !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=lC6H7                      7.24E14     -1.38       4.0E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!nC4H5+C2H2=C6H7#                       1.96E19     -3.35       5.2E3 !
<WESTMORELAnD89, p=2.6kPa>!
nC4H5+C2H2=C6H7#                      7.12E21     -3.64       6.3E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H7+R1H               8.28E-28    11.89       5.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H7+R1H              3.55E-43    16.16      -0.2E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=lC6H8                   2.90E15     -0.78       1.0E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=lC6H8                  1.50E13     -0.075      0.1E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H8#                   5.50E15     -1.67       1.5E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H8#                  8.53E13     -1.11       0.8E3 !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+nC4H5=C6H6#+H2                2.80E-7      5.63      -1.9E3 !
<WESTMORELAnD89, p=2.6kPa>!
R10C2H3V+nC4H5=C6H6#+H2               1.84E-13     7.07      -3.6E3 !
<WESTMORELAnD89, p=101kPa>!
!***
nC4H5+R2OH=C4H4+H2O                    2.5E12       0.0          0.0  !
<WAnG97>!

!nC4H5+O2=R5CHO+C2H3CHO                 1.7e29      -5.31       6.5E3 !MF
as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>
nC4H5+O2=R5CHO+C2H3CHO                5.67E28      -5.31       6.5E3 !MF
nC4H5+O2=C2H4Z+B2CO+R5CHO             1.13e29      -5.31       6.5E3 !MF
nC4H5+O2=C4H4+R3OOH                   5.19E15       -1.26        3.31e3  !
MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>
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 !****** REACTIONS DE iC4H5  ***** (CH2//CHCґ//CH2) *****stablilise par
resonnance
iC4H5=nC4H5                          1.5E13       0.0        67.8E3 !
<LEUnG95>!


iC4H5(+M)=R1H+C4H4(+M)               1.0E14       0.0        50.0E3 !
<MILLER92>!
            LOW   /2.0E15 0.0 42000/
iC4H5+R1H=C4H4+H2                    3.0E13       0.0           0.0  !
<WAnG97>!
iC4H5+R4CH3=iC5H8                    1.0E13       0.0           0.0  !
<estimated> !
2R10C2H3V=iC4H5+R1H                  1.5E30      -4.95       13.0E3  !
<WAnG97>20Torr!
!***2R10C2H3V=iC4H5+R1H              1.2E22      -2.44       13.7E3  !
<WAnG97>760Torr!
iC4H5+R2OH=C4H4+H2O                  5.50E12      0.0           0.0  !
<WAnG97>!
iC4H5+O2=HCHO+CH2CHCO                4.5E16      -1.39         1.0E3  !
estimй par{O2+C2H3=HCHO+CHO}!
iC4H5+O2=C4H4+R3OOH                  1.34E6       1.61          -400  !
estimй par {O2+C2H3=C2H2+OOH}!


!****** REACTIONS DE C4H5-1s  ***** (CH3/CHґ/C///CH) *****stablilise par
resonnance

!C4H5-1s=R1H+C4H4                      3.0E13       0.0        45.0E3 !
<HIDAKA96>!
C4H5-1s=R1H+C4H4                       6.0E13       0.0        50.4E3 !
add inverse!
! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-1s+R1H=C4H4+H2                    2.0E13       0.0         0.0   !
<MILLER92/BRAUn89>!
C4H5-1s+B1O=R9C2H+CH3CHO               1.4E14       0.0         0.0   !
<MILLER92/SLAGUE91>!
C4H5-1s+R2OH=C4H4+H2O                  2.0E13       0.0         0.0   !
<MILLER92>!
C4H5-1s+R2OH=R5CHO+sC3H5               4.0E13       0.0         0.0   !
<WAnG97>!
C4H5-1s+O2=R5CHO+B2CO+C2H4Z            3.0E10       0.0         2.9E3 !
<MILLER92/SLAGUE88>!
C4H5-1s+C4H5-1s=C8H10#                 1.0E12       0.0         0.0   !
<STEIn90>shocktube!

!****** REACTIONS DE C4H5-1p  ***** (CH2ґ/CH2/C///CH) *****

!C4H5-1p=R1H+C4H4                       3.0E13       0.0        45.0E3 !
<HIDAKA96>!
!C4H5-1p=R1H+C4H4                       4.0E13       0.0        38.8E3 !
<HIDAKA96>!
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C4H5-1p=R9C2H+C2H4Z                      2.0E14       0.0        57.0E3 !
<HIDAKA96>!
C4H5-1p+O2=C4H4+R3OOH                    1.6E12       0.0         5.0E3 !
PAG00!
C4H5-1p=C4H5-1s                          5.0E12       0.0        37.4E3 !
PAG00!

!****** REACTIONS DE C4H5-2  ***** (CH3/C///C/CH2Ґ) *****stablilise par
resonnance

!C4H5-2=R1H+tC4H4                        3.0E13       0.0        50.0E3 !
<fromHIDAKA96+5!
C4H5-2=R1H+tC4H4                         6.0E13       0.0        54.3E3 !
toto!

!C4H5-2=iC4H5                            3.0E13       0.0        50.0E3 !
<fromHIDAKA96>!
C4H5-2=iC4H5                             5.0E12       0.0        50.5E3 !
PAG00!
C4H5-2+C4H5-2=C8H10#                     1.0E12       0.0           0.0 !
<STEIn90>shocktube!

! Les rйactions suivantes sont deduites de celles de C3H3
C4H5-2+B1O=C3H3+HCHO                   1.4E14       0.0          0.0   !
<MILLER92/SLAGUE91>!
C4H5-2+R2OH=R10C2H3V+B2CO+R4CH3        4.0E13       0.0          0.0   !
<WAnG97>!
C4H5-2+O2=CH2COZ+B2CO+R4CH3            3.0E10       0.0          2.9E3 !
<MILLER92/SLAGUE88>!


!****** REACTIONS DE C4H6Z2  ***** 1,3 Butadiene (CH2CHCHCH2) *****!
!R10C2H3V+R10C2H3V=C4H6Z2              6.8E12       0.0          0.0   !
<TSAnG86 P=2.6KPa T=1500>!
R10C2H3V+R10C2H3V=C4H6Z2              9.8E14      -0.5          0.0   !
<HIDAKA96shocktube>!
!
C4H6Z2=C4H4+H2                         2.5E15       0.0       94.7E3   !
<HIDAKA96>
C4H6Z2=iC4H5+R1H                      1.4E15       0.0       98.0E3   !
<HIDAKA96>!
!
C2H4Z+R10C2H3V=C4H6Z2+R1H             5.0E11       0.0        7.3E3   !
<TSAnG86>!
!
C4H6Z2+R1H=nC4H5+H2                    1.3E6        2.53      12.2E3   !
<WAnG97>!
C4H6Z2+R1H=iC4H5+H2                    6.6E5        2.53       9.2E3   !
<WAnG97>!
!
!C4H6Z2+R1H=C4H7-1                2.6E13       0          3.2E3   !
ESTIMATED *2!
!C4H6Z2+R1H=C4H7Y                 2.6E13       0         1.56E3   !
ESTIMATED *2!
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C4H6Z2+R1H=C4H7-1                    1.3E13       0         3.2E3   !
ESTIMATED
C4H6Z2+R1H=C4H7Y                     1.3E13       0        1.56E3   !
ESTIMATED !
!
C4H6Z2+R4CH3=nC4H5+CH4                7.0E13       0.0      18.5E3   !
<WU87>!
C4H6Z2+R4CH3=iC4H5+CH4                7.0E13       0.0      15.5E3   !
<WU87-3kcal>!
!C4H6Z2+R4CH3=C5H9Y                6.3E10       0.0      7.49E3   ! PERRIN
88 nist!
!C4H6Z2+R4CH3=iC5H9                1.8E11       0.0       8.0E3   !
Estimated*2!
C4H6Z2+R4CH3=C5H9Y                   6.31E10      0.0      7.49E3   !
PERRIN 88 nist!
C4H6Z2+R4CH3=iC5H9                   9.64E10      0.0       8.0E3   !
Estimated!
!
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z          5.0E14       0.0      22.8E3   !
<HIDAKA96>!
C4H6Z2+R10C2H3V=iC4H5+C2H4Z          5.0E14       0.0      19.8E3   !
<HIDAKA96-3kcal>!
!
C4H6Z2+B1O=C3H5Y+R1H+B2CO             6.0E08       1.45      0.9E3   !
<LEUnG95,BREZInSKY84>!
!
R10C2H3V+C4H6Z2=C6H8#+R1H            7.4E014     -0.66     8.42E3   !
<frenklach >!
!R10C2H3V+C4H6Z2=C6H8#+R1H            2.28E12     -0.24      9.9E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H8#+R1H             4.15E-11     6.39      2.4E3   !
<WESTMORELAnD89, p=101kPa>!
!***
!R10C2H3V+C4H6Z2=lC6H8+R1H            1.0E10       1.05     14.0E3     !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H8+R1H             2.48E-15     8.20      6.3E3    !
<WESTMORELAnD89, p=101kPa>!
!***
C4H6Z2+C2H2=C6H8#                     2.3E12       0.0      35.0E3     !
<WESTMORELAnD89>!
!***
!MF car lC6H9 n'intervient qu'ici
!R10C2H3V+C4H6Z2=lC6H9                5.48E28     -5.31      9.3E3     !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=lC6H9                 1.48E12     -0.17      3.2E3    !
<WESTMORELAnD89, p=101kPa>!
!***
R10C2H3V+C4H6Z2=C6H9Z#               1.64E29     -6.12      9.6E3   !
<WESTMORELAnD89, p=2.6kPa>!
!R10C2H3V+C4H6Z2=C6H9Z#                7.06E13     -1.35      4.0E3   !
<WESTMORELAnD89, p=101kPa>!
!***
C4H6Z2+C2H4Z=C6H10#                   2.3E10       0.0      27.0E3   !
<WESTMORELAnD89>!
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C4H6Z2+R2OH=nC4H5+H2O                6.2E6        2.0        3.4E3     !
<WAnG97>!
C4H6Z2+R2OH=iC4H5+H2O                3.1E6        2.0        0.4E3     !
<WAnG97>!
C4H6Z2+R2OH=C3H5Y+HCHO               2.8E12       0.0       -0.9E3     !
<LInSTEDT96>!
C4H6Z2+R2OH=CH3CHO+R10C2H3V          5.6E12       0.0       -0.9E3     !
<fromLInSTEDT96>!
C4H6Z2+O2=iC4H5+R3OOH                4.0E13       0.0       57.9E3     !
<LEUnG95>!
C4H6Z2+C3H3=nC4H5+aC3H4              1.0E13       0.0       22.5E3     !
<HIDAKA96>!
C4H6Z2+C3H3=iC4H5+aC3H4              1.0E13       0.0       19.5E3     !
<HIDAKA96-3kcal>!

!****** REACTIONS DE C4H6-12  ***** (1,2) Butadiene (CH2CCHCH3) *****

!C4H6-12=C4H6Z2                      3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-12=iC4H5+R1H                   4.2E15       0.0        92.6E3 !
<LEUnG95>!
!C4H6-12+R1H=R10C2H3V+C2H4Z          4.0E11       0.0           0.0 !
<LEUnG95>!
!C4H6-12=C3H3+R4CH3                  7.3E14       0.0        75.4E3 !
<kingas1500K>!
!C4H6-12+R1H=C4H7-2                  1.3E13       0.0         1.6E3 !
<heyberger> !
!C4H6-12+R1H=C4H7Y                   1.2E11       0.69        3.0E3 !
<heyberger>!
!C4H6-12+R1H=C4H7T                   1.3E13       0.0         3.2E3 !
<heyberger> !
!C4H6-12+R1H=iC4H5+H2                1.7E5        2.5         2.5E3 !
<asTSAnG91>!
!C4H6-12+R4CH3=iC4H5+CH4             2.2E0        3.5         5.7E3 !
<asTSAnG91>!
!C4H6-12+R11C2H5=iC4H5+C2H6          2.2E0        3.5         6.6E3 !
<asTSAnG91>!
!C4H6-12+B1O=iC4H5+R2OH              1.7E11       0.7         5.9E3 !
<asTSAnG91>!
!C4H6-12+R2OH=iC4H5+H2O              3.1E6        2.0        -0.3E3 !
<asTSAnG91>!
!C4H6-12+R3OOH=iC4H5+H2O2            9.6E3        2.6        13.9E3 !
<asTSAnG91>!


!****** REACTIONS DE (c-C4H6)  ***** methyl-cyclopropene  *****

!B6CH2+pC3H4=cC4H6                    1.8E14       0.0         0.0   !
<LEUnG95>!
!cC4H6=C4H6Z2                        3.0E13       0.0        42.3E3 !
<LEUnG95>!
!cC4H6=C4H6-12                       3.0E13       0.0        43.8E3 !
<LEUnG95>!
```

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!****** REACTIONS DE (C4H6-1) *****  1 Butyne *****

!C4H6-1=C4H6-12                          2.5E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-1=C4H5-1s+R1H                      7.7E14       0.0        87.9E3 !
Kinga&dH Melius!
!C4H6-1=C4H5-1p+R1H                      9.1E14       0.0        99.6E3 !
Kingas!
!C4H6-1=>C3H3+R4CH3                     3.0E15       0.0        75.8E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                 1.3E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R11C2H5+C2H2                6.5E4        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-1+R1H=R4CH3+aC3H4                  3.2E12       0.0         1.7E3 !
<asWAGnER72>!
!C4H6-1+R1H=R11C2H5+C2H2                 3.2E12       0.0         1.7E3 !
<asWAGnER72>!
! Les rйactions suivantes sont deduites de celles de 1-C4H8 generes par
EXGAS
!C4H6-1+R1H=H2+C4H5-1s                   5.4E4        2.5        -1.9E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1s                1.5E12       0.0         7.1E3 !
<EXGAS>!
!C4H6-1+B1O=R2OH+C4H5-1s                 8.8E10       0.7         3.2E3 !
<EXGAS>!
!C4H6-1+R2OH=H2O+C4H5-1s                 3.0E6        2.0        -1.5E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1s               1.4E12       0.0        36.0E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s                1.4E12       0.0        41.4E3 !
<InGHAM95sec>!
!C4H6-1+O2=>R3OOH+C4H5-1s               4.2E12       0.0        49.5E3 !
<DAGAUT90sec>!
!C4H6-1+R3OOH=>H2O2+C4H5-1s              6.4E3        2.6        12.4E3 !
<EXGAS>!
! Les rйactions suivantes sont deduites de celles generes par EXGAS pour
H primaires
!C4H6-1+R1H=H2+C4H5-1p                   2.9E7        2.0         7.7E3 !
<EXGAS>!
!C4H6-1+R4CH3=CH4+C4H5-1p                3.7          4.0         8.2E3 !
<EXGAS>!MF
!C4H6-1+B1O=R2OH+C4H5-1p                 5.1E13       0.0         7.8E3 !
<EXGAS>!
!C4H6-1+R2OH=>H2O+C4H5-1p                2.7E6        2.0        -0.4E3 !
<EXGAS>!
!C4H6-1+O2=>R3OOH+C4H5-1p                1.2E13       0.0        49.0E3 !
<EXGAS>!
!C4H6-1+R3OOH=>H2O2+C4H5-1p              6.0E11       0.0        17.0E3 !
<EXGAS>!
! Les rйactions d'addition suivantes sont deduites de celles de pC3H4
!C4H6-1+B1O=R12CHCOZ+R11C2H5             1.5E13       0.0         2.1E3 !
<asWARnATZ84>!
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!C4H6-1+R2OH=CH2COZ+R11C2H5           4.3E11       0.0        -0.8E3 !
<asBOODAGHIAnS87>!

!***** REACTIONS DE (C4H6-2)***** 2 Butyne  *****

!C4H6-2=C4H6Z2                        3.0E13       0.0        65.0E3 !
<HIDAKA96>!
!C4H6-2=C4H6-12                       3.0E13       0.0        67.0E3 !
<HIDAKA96>!
!C4H6-2=C4H5-2+R1H                    2.0E14       0.0        87.3E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4              2.6E5        2.5         1.0E3 !
<HIDAKA96>!
!C4H6-2+R1H=R4CH3+pC3H4               6.5E12       0.0         1.7E3 !
<asWAGnER72>


! Les rйactions suivantes sont deduites de celles de pC3H4
!C4H6-2+R1H=C4H5-2+H2                 3.4E5        2.5          2.5E3 !
<asTSAnG91*2>!
!C4H6-2+R4CH3=C4H5-2+CH4              4.4E0        3.5          5.7E3 !
<asTSAnG91*2>!
!C4H6-2+B1O=B2CO+R10C2H3V+R4CH3       1.5E13       0.0          2.1E3 !
<asWARnATZ84>!
!C4H6-2+B1O=R2OH+C4H5-2               1.2E11       0.7          7.6E3 !
<asTSAnG91*2>!
!C4H6-2+R2OH=B2CO+C2H4Z+R4CH3         4.3E11       0.0         -0.8E3 !
<asBOODAGHIAnS87>!
!C4H6-2+R2OH=C4H5-2+H2O               6.2E6        2.0         -0.3E3 !
<asTSAnG91*2>!
!C4H6-2+O2=C4H5-2+R3OOH               4.2E12       0.0         44.0E3 !
<InGHAM95*2>+4!
!C4H6-2+R3OOH=C4H5-2+H2O2             1.9E4        2.6         13.9E3 !
<asTSAnG91*2>!


!******* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y                         3.34E09       1.0       39.1E3  !
ESTIMATED !
!C4H7-1=C4H7V                         3.3E9         1.0       20.7E3  !
Estimated!
!C4H7-1=C2H4Z+R10C2H3V                2.0E13        0.0       35.5E3  !
Estimated!
!C4H7-1+R4CH3=C5H10                   2.0E13        0.0          0.0  !
Estimated !
!C4H7-1+R1H=C4H8Y                     1.0E14        0.0          0.0  !
Estimated!

!******* Reactions de C4H7Y (CH3-CH.-CH=CH2)!*****stablilise par
resonnance
!C4H7Y+R1H=C4H8Y                      2.0E13        0.0          0.0  !
asTSANG 91!!
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!C4H7Y+R1H=H2+C4H6Z2                    0.9E13        0.0         0.0  !
asTSANG 91!!
!C4H7Y+R1H=H2+C4H6-12                   0.9E13        0.0         0.0  !
asTSANG 91!
!C4H7Y+R3OOH=R2OH+C2H3CHO+R4CH3        1.0E15       -0.8         0.0  !
<Heyberger>!
!C4H7Y+R4CH3=iC5H10                     0.5E13        0.0         0.0  !
Estimated !

!**************Reactions de C4H7V (CH3-CH2-CH=CH.)*******!
!C4H7V=C4H7Y                           1.9E10         1.0      36.3E3  !
Heyberger!
!C4H7V=R11C2H5+C2H2                    2.0E13         0.0      33.0E3  !
Heyberger!

!**************Reactions de C4H7-2 (CH3-C.=CH-CH3)*****!
!C4H7-2=C4H7Y                          2.9E10     1.0        37.8E3  !
ESTIMATED !
!C4H7-2=R4CH3+pC3H4                    2.0E13      0.0     31.5E3  !
ESTIMATED !

!**************Reactions de C4H7T (CH2=C.-CH2-CH3)********!

!C4H7T=C4H7-1                          3.34E09      1.0      40.6E3   !
ESTIMATED !
!C4H7T=C4H7Y                           2.0E13       0.0      47.0E3   !
<Heyberger>!
!C4H7T=R4CH3+aC3H4                     2.0E13       0.0      32.5E3   !
ESTIMATED !

!**************Reactions du 1-butene!

!C4H8Y+O2=C4H7Y+R3OOH                  3.6E12       0.0        38.2E3  !
<Heyberger>!
!C4H8Y+R1H=C4H7Y+H2                    5.4E4        2.5        -1.9E3  !
<Heyberger>!
!C4H8Y+R2OH=>HCHO+R4CH3+C2H4Z          1.4E12       0.0        -1.0E3  !
<Heyberger>!
!C4H8Y+R2OH=R4CH3+C2H5CHO              1.4E12       0.0        -1.0E3  !
<Heyberger>!!ds мйса PRF
!C4H8Y+R2OH=R4CH3+C2H5CHO        6.800E+11   0.0    -928.0 !(89ATK*RTi)
!C4H8Y+R2OH=C4H7Y+H2O                  3.0E6        2.0       -1.52E3  !
<Heyberger>!
!C4H8Y+R4CH3=C4H7Y+CH4                 1.0E11       0.0         7.3E3  !
<Heyberger>!

!C2H5CHO+R1H=H2+B2CO+R11C2H5           4.0E13       0.0        4.2E3  !
<Heyberger>!
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5         4.0E12       0.0        0.5E3  !
<Heyberger>!

!***********reactions de iC4H8********!
!iC4H8+R2OH=iC3H7+HCHO                  1.4E12       0.0     -1040.0    !
(idem RF)
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!iC4H8+R1H=>iC4H7+H2                    3.5E5        2.5        2510    !
(idem RF)
!iC4H8+R2OH=>iC4H7+H2O                  6.0D+06    2.000      -298.0    !
MES 878<C.M.>!(idem RF)
!iC4H7+R1H=iC4H8                       1.0E14       0.0         0.0    !
<estimation>!
!iC4H7+R3OOH=>R2OH+HCHO+tC3H5           1.0E15      -0.8         0.0    !
<Heyberger>!


!
**********************************************************************
**!
!
**********************************************************************
*********!
!*              MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE
*!
!*
*!
!*    efficiency  coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
**********************************************************************
*********!
!*           PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
**********************************************************************
*********!


!REACTIONS OF BENZENE MOLECULES!
!***Umimolecular inititiation!
C6H5#+R1H(+M)=C6H6#(+M)              1.0E14      0.0        0.0      !
<WANG97>!
                          LOW   /6.6E75  -16.3   7.0E3/
                          TROE /1.0 0.1 585 6113/
      O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
!***Bimolecular inititiation!
C6H6#+O2=C6H5#+R3OOH                6.0E13      0.0          63.4E3   !
<ALZUETA00>!
!***additions!
C6H6#+R1H=C6H7#                      3.2E13      0.0         3.2E3   !
<MEBEL97>!
C6H6#+B1O=C6H5O#+R1H                 2.8E13      0.0        4.91E3   !
<EMDEE92>!
C6H6#+R2OH=C6H5OH#+R1H               1.3E13      0.0        10.6E3   !
<BAULCH94>!
C6H6#+R9C2H=C6H5#C2H+R1H             5.0E13      0.0           0.0   !
<WANG97>!
C6H6#+R10C2H3V=styrene+R1H           7.9E11      0.0         6.4E3   !
<WANG97>!
!***Metatheses!
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!*modif Zhenyu*!
!C6H6#+R1H=C6H5#+H2                  6.0E8       1.8         16.8E3   !
<MEBEL97>!
C6H6#+R1H=C6H5#+H2                   1.22E8      2.031      15.88E3   !
calcul CBS-QB3 Fournet

C6H6#+B1O=C6H5#+R2OH              2.0E13    0.0         14.7E3   !
<LINDSTEDT94>!

!*modif Zhenyu*!
!C6H6#+R2OH=C6H5#+H2O                1.6E8       1.42        1.45E3   !
<BAULCH92>!
C6H6#+R2OH=C6H5#+H2O                  1.36E4      2.7       0.6196E3   !as
toluene+R2OH=C6H4CH3+H2O

!*modif Zhenyu*!
!C6H6#+R3OOH=C6H5#+H2O2              5.5E12      0.0         28.9E3   !
<BAULCH94>!
C6H6#+R3OOH=C6H5#+H2O2               9.2E12      0.0        28.81E3   !as
toluene+R3OOH=C6H4CH3+H2O2

!*modif Zhenyu*!
!C6H6#+R4CH3=C6H5#+CH4                2.0E12      0.0         15.0E3   !
<ZHANG89>!
C6H6#+R4CH3=C6H5#+CH4                2.07E0      3.861       13.3E3   !
calcul CBS-QB3 Fournet

C6H6#+R11C2H5=C6H5#+C2H6             6.3E11      0.0         15.0E3   !
<ZHANG89>!
C6H5#+C3H6Y=C6H6#+C3H5Y              7.94E13     0.0        11.94E3   !MF
<Heckmann,Hippler,Troe(1996)>
C6H6#+nC4H5=C6H5#+C4H6Z2             6.3E11      0.0         15.0E3   !
estimated!
C6H6#+iC4H5=C6H5#+C4H6Z2             6.3E11      0.0         20.0E3   !
estimated!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=lC6H7                          2.5E14      0.7        41.8E3    !
<WEISSMAN89!

!***Decomposition by beta-scission!
!C6H7#=>C2H2+nC4H5                   2.0E13      0.0        50.0E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
HEYBERGER02!
!***Oxidation!
C6H7#+O2=C6H6#+R3OOH                 7.9E11      0.0         9.9E3    !
estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combimations!
C6H7#+R1H=C6H8#                      1.0E14      0.0         0.0      !
estimated!
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!***Disproportionnations!
C6H7#+R1H=C6H6#+H2                  3.3E12      0.0        0.0      !
<RISTORI01>!
C6H7#+R2OH=C6H6#+H2O                1.0E13      0.0        0.0      !
estimated!
C6H7#+R4CH3=C6H6#+CH4               3.0E12     -0.32      -0.1E3    !
estimated!
C6H7#+C6H7#=C6H6#+C6H8#             8.4E10      0.0       -0.3E3    !
estimated!
!analogy with the disproprotionnations ofC3H5Y proposed by TSANG91!

!REACTIONS OF C6H5# RADICALS!
!***Isomerization!
C6H5#=lC6H5                         5.0E13      0.0       72.5E3    !
<BRAUN89>!
!lC6H5 = ch///c/ch//ch/ch//ch(.)!
lC6H5=>2C2H2+R9C2H                   2.0E13      0.0       51.0E3   !
estimated!
!DH298 =44kcal/mol, Eadd=7 kcal/mol!
lC6H5=lC6H4+R1H                          2.0E12      0.0
41.0E3   !estimated!
!lC6H4 = ch///c/ch//ch/c///ch , DH298 =38kcal/mol, Eadd=3 kcal/mol!
!from BRAUN89 at 1500 K!
!***Reactions with O2!
C6H5#+O2=C6H5O2                     2.2E19     -2.5         0.0    !
estimated!

C6H5#+O2=C6H5O#+B1O                 2.6E13      0.0        6.1E3    !
<FRANK94>!
C6H5#+O2=OC6H4O+R1H                 3.0E13      0.0        9.0E3    !
<FRANK94>!


!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!
!***Additions!
C6H5#+C2H2=C6H5#C2H+R1H             4.0E13      0.0       10.1E3    !
<MARINOV97>!
C6H5#+C6H6#=biphenyl+R1H            5.6E12     -0.074      7.5E3    !
<WANG97>!
!***Combinations!
C6H5#+B1O=C5H5#+B2CO               1.0E14      0.0          0.0     !
<FRANK94>!
C6H5#+R2OH=C6H5OH#                    1.0E13       0.0          0.0
!calculated!
!toluene=C6H5#+R4CH3                  1.0E16       0.0         97.0E3
!<COLKET94>!
!calculation by KINGAS!
C6H5#+R5CHO=C6H5CHO                 5.0E12      0.0        0.0      !
estimated!
C6H5#+R10C2H3V=styrene              5.0E12      0.0        0.0      !
estimated!
C6H5#+R11C2H5=etC6H5                5.0E12      0.0        0.0      !
estimated!
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C6H5#+R3OOH=C6H5O#+R2OH              5.0E12      0.0         0.0      !
estimated!
!C6H5C3H3 n'intervient qu'ici
!C6H5#+C3H3=C6H5C3H3                  3.0E12      0.0         0.0      !
<D'ANNA98>!
C6H5#+C6H5#=biphenyl                 3.8E31     -5.75        7.9E3    !
<WANG97>!
!***disproportionnations!
C6H5#+R2OH=C6H5O#+R1H                5.0E13      0.0         0.0      !
<ALZUETA00>!
C6H5#+C6H7#=C6H6#+C6H6#              1.0E12      0.0         0.0      !
<SHANDROSS96>!

!REACTIONS OF PHENYLPEROXY RADICALS!
!***Decomposition by beta-scission!
!mfC6H5O2=OC6H4O+R1H                    2.0E13      0.0        30.0E3    !
estimated!
C6H5O2=C5H4O#+R5CHO                  2.0E13      0.0        30.0E3    !
estimated!
!see DA COSTA01!

!MF
C6H5O2+R3OOH=C6H5OOH+O2                    2.0E11          0.00  -1300
C6H5OOH=C6H5O#+R2OH                        1.5E16         0.00   43000


!REACTIONS OF PHENOXY RADICALS!
!***CO elimination!
C6H5O#=B2CO+C5H5#                     2.5E11      0.0       43.8E3    !
<BAULCH92>!
!***Combinations!
!--C6H5O#+R1H(+M)=C6H5OH#(+M)         2.5E14      0.0         0.0     !
<FRENKLACH>!
C6H5O#+R1H(+M)=C6H5OH#(+M)           1.0E14      0.0         0.0     !
estimated!
                           LOW   /1.0E94  -21.84   13.9E3/           !
<FRENKLACH>!
                           TROE /0.043 304 60000 5896/
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/
C6H5O#+R1H=C5H6#+B2CO                1.1E53    -10.7         41.4E3   !
<TAN96>!
C6H5O#+B1O=OC6H4OH                    2.6E10      0.47         0.8E3   !
<LIN95>!
C6H5O#+B1O=OC6H4O+R1H                 8.5E13      0.0          0.0     !
<FRANCK94>!
C6H5O#+B1O=C5H5#+CO2                  1.0E13      0.0          0.0     !
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!
!***CO elimination!
OC6H4OH=B2CO+C5H4OH#                  7.4E11      0.0         43.8E3   !
estimated!
!as for phenoxy radicals!
```

```
!REACTIONS OF CYCLOPENTADIENYL RADICALS!
!***Isomerization!
C5H5#=lC5H5                          1.0E14      0.0       45.5E3    !
<BRAUN89>!

!lC5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car lC5H6 n'intervient qu'ici
!lC5H5+R1H=lC5H6                     1.0E14      0.0        0.0      !
estimated!
lC5H5=C3H3+C2H2                     2.0E13      0.0        50.0E3   !
estimated!
!DH298 =43kcal/mol, Eadd=7 kcal/mol!


!***Reactions with O2!
C5H5#+O2=R5CHO+C4H4O                1.2E19     -2.48      11.0E3    !
<ZHONG98>!
!***Combinations!
C5H6# = C5H5# + R1H                          5.0E15          0.00   7.87E4
     ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>

C5H5#+B1O=C5H4O#+R1H                5.8E13     -0.02       0.02E3   !
<ZHONG98>!
C5H5#+B1O=>2C2H2+R5CHO              3.2E13     -0.17       0.44E3   !
<ZHONG98>!
C5H5#+R2OH=>C4H6Z2+B2CO              4e14       0.0         4500 !
[PENGLOAN- RODA]


C5H5#+R2OH=C5H5OH#                 1.0E13      0.0        0.0      !
calculated!
C5H5#+R3OOH=C5H5O#+R2OH              3.0E12      0.0        0.0      !
calculated!
!calculation by KINGAS!
C5H5#+C5H5#=>C10H10#                 2.0E12      0.0        0.0      !
estimated!
C10H10#=>C5H5#+C5H5#                 3.2E15      0.0        57.5E3   !
calculated!
!***disproportionnations!
C5H5#+R3OOH=>C5H6#+O2                2.5E9       1.0        3.5E3    !
estimated!
!estimated as for allylic radicals (HEYBERGER02)/10!

!REACTIONS OF CYCLOPENTADIONYL RADICALS!
!***Decompositions by beta-scission!
C5H5O#=>2C2H2+R5CHO                   2.0E13      0.0       30.0E3   !
estimated!
C5H5O#=C5H4O#+R1H                    2.0E13      0.0       30.0E3   !
estimated!
!see DA COSTA01!
!***Combinations!
C5H5O#+R1H=C5H5OH#                   1.0E14      0.0        0.0      !
estimated!
```

```
!***no disproportionnations considered!

!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!
C5H4OH#+O2=C5H4O#+R3OOH              1.0E13      0.0        5.0E3    !
estimated!
C5H4OH#+R1H=C5H5OH#                  1.0E14      0.0        0.0      !
estimated!
C5H4OH#+B1O=CO2+C2H2+R10C2H3V        3.2E13     -0.17       0.44E3   !
estimated!
!C5H4OH#+R3OOH=>R2OH+CO2+R10C2H3V+C2H2 3.0E12      0.0        0.0      !
estimated!
C5H4OH#+R3OOH=>R2OH+R2OH+C5H4O# 3.0E12      0.0        0.0      ! mf

C5H4OH#+R3OOH=>C5H5OH#+O2            2.5E9       1.0        3.5E3    !
estimated!
!Reactions derived from those of cyclopentadienyl radicals!
C5H4OH#+C6H5O#=C5H4O#+C6H5OH#        1.0E12      0.0        0.0      !
estimated!


!
*************************************************************************
*********!
!*
!*                    SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!*
!
*************************************************************************
*********!

!REACTIONS OF ORTHOBENZOQUINONE!
OC6H4O=>C5H4O#+B2CO                  1.0E12      0.0       40.0E3    !
<ALZUETA00>!
OC6H4O+R1H=>2B2CO+C2H2+R10C2H3V      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
!OC6H4O+R1H=>H2+2B2CO+C2H2+R9C2H      1.6E6       2.5        9.8E3    !
estimated!
!OC6H4O+R2OH=>H2O+2B2CO+C2H2+R9C2H    4.4E6       2.0        1.4E3    !
estimated!
!estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!
C6H5OH#=C5H6#+B2CO                   1.0E12      0.0        61.2E3   !
<HORN98>!


C6H5OH#+O2=R3OOH+C6H5O#              1.0E13     0.0       38.9E3    !
<ALZUETA00>!


C6H5OH#+B1O=OC6H4OH+R1H              1.6E13     0.0         3.4E3    !
estimated!
```

```
!as the addition of O-atoms to toluene (DACOSTA01)!
C6H5OH#+R1H=C6H5O#+H2                1.2E14     0.0       12.4E3    !
<ALZUETA00>!
C6H5OH#+B1O=C6H5O#+R2OH              1.3E13     0.0        2.9E3  !
<ALZUETA00>!
C6H5OH#+R2OH=C6H5O#+H2O              1.4E8      1.4       -0.96E3  !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H5O#+H2O2            1.0E12      0.0       10.0E3    !
<ALZUETA00>!
C6H5OH#+R4CH3=C6H5O#+CH4             1.8E11      0.0        7.7E3    !
<MULCAHY65>!
C6H5OH#+C6H5#=C6H5O#+C6H6#           4.9E12      0.0        4.4E3    !
<ALZUETA00>!
!C6H5OH#+C5H5#=C6H5O#+C5H6#          4.9E11          0.0        9.4E3    !
estimated!
!C6H5OH#+C3H5Y=C6H5O#+C3H6Y          4.9E11     0.0        9.4E3    !
estimated!
!C6H5OH#+iC4H5=C6H5O#+C4H6Z2         4.9E11          0.0        9.4E3    !
estimated!
C6H5OH#+C5H5#=C6H5O#+C5H6#           2.67e14         0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+C3H5Y=C6H5O#+C3H6Y          2.67e14     0.0        25.238e3    !mf
<Lovell Int. J. Chem. Kinet.21(1989)547>
C6H5OH#+iC4H5=C6H5O#+C4H6Z2          2.67e14         0.0        25.238e3
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>


!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!
C6H5OH#+R1H=C6H4OH#+H2               1.7E14      0.0       16.0E3    !
<SHANDROSS96>!
C6H5OH#+B1O=C6H4OH#+R2OH             2.0E13     0.0          14.7E3    !
estimated!
C6H5OH#+R2OH=C6H4OH#+H2O             1.4E13     0.0        4.6E3   !
<SHANDROSS96>!
C6H5OH#+R3OOH=C6H4OH#+H2O2           4.0E11      0.0       28.9E3    !
estimated!
C6H5OH#+R4CH3=C6H4OH#+CH4           2.0E12      0.0       15.0E3    !
estimated!
!as the H-abstractions from benzene!

C6H4OH#+O2=OC6H4OH+B1O                2.1E13      0.0       6.1E3    !
estimated!
!as for phenyl radicals (FRANCK94)!
C6H4OH#+R1H=C6H5OH#                   1.0E14      0.0       0.0      !
estimated!
C6H4OH#+R4CH3=HOC6H4CH3               5.0E12      0.0       0.0      !mf


!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!
C5H6#+O2=>C5H5#+R3OOH                1.4E12      0.0        31.6E3   !
<INGHAM94>!
!C5H6#+R1H=C5H7#                      5.2E13      0.0        3.2E3    !
estimated!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!
```

```
C5H6#+B1O=>C5H5O#+R1H                  8.9E12     -0.15       590.0    !
<ZHONG98>!
C5H6#+R1H=C5H5#+H2                    2.8E13      0.0         2.0E3    !
<ROY97>!
C5H6#+B1O=C5H5#+R2OH                  4.8E4       2.7         1.1E3    !
<ZHONG98>!
C5H6#+R2OH=C5H5#+H2O                  3.1E6       2.0         0.0      !
<ZHONG98>!
C5H6#+R3OOH=C5H5#+H2O2                1.1E4       2.6        12.9E3    !
<ZHONG98>!
C5H6#+R4CH3=C5H5#+CH4                 1.8E-1      4.0         0.0      !
<ZHONG98>!
C5H6#+C3H5Y=C5H5#+C3H6Y              1.6E12       0.0        15.1E3    !
astoluene!
C5H6#+nC4H5=C5H5#+C4H6Z2              1.6E12      0.0        11.1E3    !
astoluene!
C5H6#+iC4H5=C5H5#+C4H6Z2              1.6E12      0.0        15.1E3    !
astoluene!
!C5H6#+C3H5Y=C5H5#+C3H6Y              6.0E12      0.0         0.0      !
estimated!
!C5H6#+nC4H5=C5H5#+C4H6Z2              6.0E12      0.0         0.0      !
estimated!
!C5H6#+iC4H5=C5H5#+C4H6Z2              6.0E12      0.0         0.0      !
<EMDEE92>!

!C5H7#=>C2H2+C3H5Y                    2.0E13      0.0        35.5E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by
HEYBERGER02!
!C5H7#+O2=C5H6#+R3OOH                  7.9E11      0.0         5.0E3    !
estimated!
!oxidation of an alkylic radical!

!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!
C5H4O#=>2C2H2+B2CO                      5.7E32     -6.76       68.5E3    !
<ALZUETA00>!
!C5H4O#=B2CO+C4H4                       1.00e12     0.0         53000    !
roda PENGLOAN!
C5H4O#+R1H=B2CO+nC4H5                  2.6E13      0.0         3.2E3    !
estimated!


!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!
C5H4O#+B1O=C4H4+CO2                    1.0E13      0.0         2.0E3     !
<ALZUETA00>!
C5H4O#+R1H=C5H3O#+H2                   8.13E7      2.031      15.88E3     !MF
idem C6H6#+R1H=C6H5#+H2
C5H4O#+B1O=C5H3O#+R2OH                 1.4E13      0.0        14.7E3     !
<ALZUETA00>!
C5H4O#+R2OH=C5H3O#+H2O                 1.1E8       1.42        1.4E3     !
<ALZUETA00>!

C5H3O#=>C2H2+B2CO+R9C2H                 2.0E13      0.0         51.0E3    !
estimated!
```

```
!estimated as the decomposition of lC6H5!
C5H3O#+O2=>CO2+C2H2+R12CHCOZ          9.7E58   -13.47       38.2E3    !
<ALZUETA00>!

C5H5OH#+R1H=C5H5O#+H2              4.0E13      0.0        6.1E3    !
<ALZUETA00>!
C5H5OH#+B1O=C5H5O#+R2OH              1.0E13      0.0        4.6E3    !
<ALZUETA00>!
C5H5OH#+R2OH=C5H5O#+H2O              1.0E13      0.0        1.7E3    !
<ALZUETA00>!

!Estimated from the same reaction for CH3OH!

C5H5OH#+R1H=C5H4OH#+H2                  1.4E13      0.0       2.0E3    !
estimated!
C5H5OH#+B1O=C5H4OH#+R2OH             4.8E4      2.7        1.1E3    !
estimated!
C5H5OH#+R2OH=C5H4OH#+H2O             1.5E6      2.0        0.0E3    !
estimated!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!
!additions decomposition
C4H4O+R1H=>R10C2H3V+CH2COZ            1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>C2H4Z+R12CHCOZ             1.3E13    0.0        3.0E3     !
estimated!
C4H4O+R1H=>sC3H5+B2CO                 1.3E13    0.0        1.5E3     !
estimated!
C4H4O+R2OH=>C2H3CHO+R5CHO             1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+R2OH=>CO2+C3H5Y                1.4E12    0.0       -1.0E3     !
estimated!
C4H4O+B1O=>R13CH2CHO+R12CHCOZ         6.0E4     2.56      -1.1E3     !
estimated!
C4H4O+B1O=>2CH2COZ                    6.0E4     2.56      -1.1E3     !
estimated!
!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition
C4H4O+R1H=>C2H2+R12CHCOZ+H2           8.2E5     2.5        12.3E3    !
estimated!
C4H4O+R1H=>C3H3+B2CO+H2               4.1E5     2.5         9.8E3    !
estimated!
C4H4O+R2OH=>C2H2+R12CHCOZ+H2O         2.2E6     2.0         2.8E3    !
estimated!
C4H4O+R2OH=>C3H3+B2CO+H2O             1.1E6     2.0         1.5E3    !
estimated!
C4H4O+B1O=>C2H2+R12CHCOZ+R2OH         1.2E11    0.7         8.7E3    !
estimated!
C4H4O+B1O=>C3H3+B2CO+R2OH             6.0E10    0.7         8.7E3    !
estimated!
!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!
```

```
!
!*****************************************************************************
*********!
!*                                                                 *!
!*              MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE
*!
!*                                                                 *!
!*    efficiency  coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#
and toluene*!
!*                                                                 *!
!
!*****************************************************************************
*********!

!
!*****************************************************************************
*********!
!*                                                                 *!
!*            PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE
*!
!*                                                                 *!
!
!*****************************************************************************
*********!

!*********************************!
!*REACTIONS OF TOLUENE MOLECULES*!
!*********************************!

!**UMIMOLECULAR INITITIATIONS


toluene=benzyl+R1H              2.09E15  0.0   87.51E3    !
<Oehlschlaeger07>! Zhenyu
toluene=C6H5#+R4CH3               2.66E16  0.0   97.88E3    !
<Oehlschlaeger07> Zhenyu

!**BIMOLECULAR INITITIATION
toluene+O2=benzyl+R3OOH      1.8E12   0.0    39.7E3    !<BAULCH94>!
!toluene+O2=benzyl+R3OOH      2.18e7   2.50    46045    !
mf<Oehlschlaeger06>!

!**ADDITIONS

toluene+R1H=C6H6#+R4CH3           5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet Zhenyu

toluene+B1O=OC6H4CH3+R1H      1.7E13   0.0     3.6E3    !<TAPPE89>!
!toluene+R2OH=HOC6H4CH3+R1H        2.3E12   0.0   -0.36E3   !<BAULCH92>!
toluene+R2OH=HOC6H4CH3+R1H    1.3E13   0.0    10.6E3    !<BAULCH94>as
benzene!
```

```
toluene+R2OH=C6H5OH#+R4CH3     7.83E2   2.884  3.2193E3  !Seta V Nakajima
V Miyoshi JPCA 2006 Zhenyu
!toluene+R2OH=C6H5OH#+R4CH3     1E5    2.58   1134.0    !Olive as
benzene+OH


!**METATHESES
!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

toluene+R1H=benzyl+H2         2.92E6   2.372  5.81E3   !Calcul CBS-QB3
Fournet Zhenyu
toluene+B1O=benzyl+R2OH            6.3E11   0.0       0.0   !
<HOFFMANN90>!

toluene+R2OH=benzyl+H2O            5.2E09   1.0    0.87E3   !<BAULCH94>!

toluene+R3OOH=benzyl+H2O2     4.0E11   0.0    14.0E3   !<BAULCH94>!
toluene+R4CH3=benzyl+CH4      3.91E0   3.76   6.98E3   !Calcul CBS-QB3
Fournet Zhenyu

! ajout MF
toluene+R7CH3O=benzyl+CH3OH     2.12E+10 0.0 3000.0        !PITZ2001
toluene+R8CH3OO=benzyl+CH3OOH   1.02E+04 2.5 12339.3  !PITZ2001


!toluene+R5CHO=benzyl+HCHO     3.77E13   0.0 23.7874E3    !MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO           1.26e8   1.9   18.183E3
benzyl+CH3CHO = toluene+R14CH3CO 1.26e8   1.9   18.183E3

toluene+R10C2H3V=benzyl+C2H4Z  4.0e12   0.0     8.0e3       !<COLKET94>!

toluene+C3H5Y=benzyl+C3H6Y    1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+C3H3=benzyl+pC3H4     1.6E12   0.0    15.1E3   !<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2        1.6E12   0.0    15.1E3   !
<estimated(a)>!
toluene+nC4H5=benzyl+C4H6Z2        1.6E12   0.0    11.1E3   !
<estimated(a)>!
toluene+C5H5#=benzyl+C5H6#    1.6E11   0.0    15.1E3   !<estimated(a)>!
!(a) :Rate constant taken equal to that of the H-abstraction with methyl
radicals proposed !
!by COLKETT94 with A divided by 10 for cyclic radicals !
! and with an activation energy 4 kcal/mol higher for resonnance
stabilised radicals!



!ajout MF
toluene+C6H5O2=benzyl+C6H5OOH                 1.02E+04 2.5 12339.3    !
PITZ2001


toluene+C6H5#=benzyl+C6H6#    7.9E13   0.0    12.0E3   !<HECKMANN96>!
```

```
toluene+C6H5O#=benzyl+C6H5OH#         1.6E11   0.0   15.1E3 !
<estimated(a)>! peut etre trop rapide
toluene+C6H4CH3=benzyl+toluene       7.9E13   0.0   12.0E3  !
<estimated(b)>!
toluene+OC6H4CH3=benzyl+HOC6H4CH3   1.6E11   0.0   15.1E3  !
<estimated(a)>!
toluene+C6H5CH2OO=benzyl+C6H5CH2OOH 4.0E11   0.0   14.0E3  !
<estimated(c)>!
toluene+C6H5CH2O=benzyl+C6H5CH2OH    1.6E11   0.0   11.1E3 !
<estimated(a)>!
toluene+HOC6H4CH2=benzyl+HOC6H4CH3  1.6E11   0.0   15.1E3  !
<estimated(a)>!
!(b) :Rate constant taken equal to that of the H-abstraction with phenyl
radicals proposed !
!by HECKMANN96!
!(c) :Rate constant taken equal to that of the H-abstraction with HO2
radicals proposed !
!by BAULCH94!

!**METATHESES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2          1.22E08  2.031 15.88E3  !as
C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu
toluene+B1O=C6H4CH3+R2OH   2.0E13   0.0    14.7E3     !<estimated(d)>!

toluene+R2OH=C6H4CH3+H2O     1.36E4   2.7  0.6196E3   !<Seta06>! in
Sakai07 Zhenyu
toluene+R3OOH=C6H4CH3+H2O2   9.2E12   0.0   28.81E3   !<Baulch94>! in
Sakai07 Zhenyu
toluene+R4CH3=C6H4CH3+CH4   2.07E0   3.861  13.3E3    !as
C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu


!*****************************!
!*REACTIONS OF BENZYL RADICALS*!
!*****************************!

!**DECOMPOSITION BY BETA-SCISSION
benzyl=>C5H5#+C2H2             6.0E13   0.0    70.0E3 !<Colket94>!
benzyl=>C3H3+C4H4              2.0E14   0.0    83.6E3 !<Colket94>!

!**REACTIONS WITH OXYGEN
benzyl+O2=C6H5CH2OO               4.6E11   0.0   -377.0   !<FENTER94>!
benzyl+O2=C6H5CH2O+B1O         6.3E12   0.0   40.0E3  !<BREZYNSKY84>!

!**TERMINATION REACTIONS
benzyl+B1O=C6H5#+HCHO         3.5E13   0.0      0.0   !<EMDEE92>!
benzyl+B1O=C6H5CHO+R1H             1.0E14   0.0      0.0   !
<estimated(e)>!
!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4
!(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH3OO=>C6H5CH2O+R7CH3O            5.0E12     0.0        0.0
benzyl+R17C2H5OO=>C6H5CH2O+R15C2H5O        5.0E12     0.0        0.0
```

```
benzyl+R2OH=C6H5CH2OH          2.0E13   0.0      0.0  !<HIPLER91>!

!MFbenzyl+R3OOH=C6H5CH2OOH        5.0E12   0.0      0.0    !<HIPPLER92>!
benzyl+R3OOH=C6H5CH2OOH           8.21E4   2.20      -5.13E3     !MF<da
silva-bozzelli- proceedings  comb inst 32(2009)287-294>!

2benzyl=bibenzyl                    5.01E12   0.0 0.454E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3           6.1e15    0.0   75120   !<BAULCH94>!

!************************************!
!*REACTIONS OF METHYL PHENYL RADICALS*!
!************************************!

!**reactions with oxygen
!mfC6H4CH3+O2=OC6H4CH3+B1O                 2.6E13   0.0   6.1E3  !
<estimated(f)>!
!mfC6H4CH3+O2=OC6H4O+R4CH3                 3.0E13   0.0   9.0E3  !
<estimated(f)>!
!(f) : Rate constant taken equal to that of the similar reaction in the
case of phenyl!
!radicals!

!ajout mf
C6H4CH3+O2=>OOC6H4CH3                 3.72E13         -0.22      -711
     !2008DAS/BOZ3566-3575
OOC6H4CH3=>C6H4CH3+O2                 6.36E19        -1.372     48.74E3
          !2008DAS/BOZ3566-3575
OOC6H4CH3=>OC6H4CH3+B1O                     1.27E15         -0.25
     3.85E4          !2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3                     5.0E11          0.00
     46400      !



!***termination reactions!
C6H4CH3+R1H=toluene                   1.0E14   0.0   0.0    !
<estimated(g)>!
!(g) : Rate constant taken equal to that of the recombination of H atoms
with alkyl !
!radicals as proposed by Allara!


C6H4CH3+B1O=OC6H4CH3                  1.0E14   0.0   0.0    !
<estimated(f)>!
C6H4CH3+R2OH=HOC6H4CH3                1.0E13   0.0    0.0   !
<estimated(f)>!
C6H4CH3+R4CH3=C8H10#            1.2E06   1.96   -3.7E3     !
<estimation(fbis)>!
!(fbis) : Rate constant taken equal to that of the similar reaction in
the case of phenyl!
```

```
!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH           5.0E12   0.0   0.0    !
<estimated(f)>!
C6H4CH3 +R1H = benzyl + R1H           1.0E13   0.0   0.0    !<MILLER92>!

!************************************!
!*REACTIONS OF BENZYL PEROXY RADICALS*!
!************************************!


!**isomerisation-decomposition reactions
C6H5CH2OO=C6H5CHO+R2OH                      3.4E9   1.0   37.5E3  !
<estimated(h)>!
!(h) : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 23 (4 membered transition
ring)!
!+ 14.5 (secondary allylic H-atom)!

!**Combination reactions
!MF C6H5CH2OO+R1H=C6H5CH2OOH               1.0E14   0.0   0.0E3  !
<estimated(g)>!

!**dispropotionnation reactions!
C6H5CH2OO+R3OOH=C6H5CH2OOH+O2         2.0E11   0.0   -1.3E3 !
<estimated(i)>!
2C6H5CH2OO=C6H5CH2OH+C6H5CHO+O2       1.4E10   0.0   -725.0 !
<estimated(i)>!
C6H5CH2OO+C6H5CH2OO=2C6H5CH2O+O2      6.3E10   0.0   -725.0 !
<estimated(i)>!
!(i) : Rate constant taken equal to that the disproportionnation of
peroxyalkyl radicals !
!as proposed by Warth!


! ajout MF
C6H5CH2OO+R1H=C6H5CH2O+R2OH                      3.80E14         -0.19
     1.89E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=C6H5CH2OOH              4.35e60         -15.92     11.40E3
     !<da silva J Chem Theory Comput 2009>
C6H5CH2OO+R1H=benzyl+R3OOH                  1.96E4          2.47  1.43E3
     !<da silva J Chem Theory Comput 2009>


!************************************!
!*REACTIONS OF BENZYL ALCOXY RADICALS*!
!************************************!

!**Decomposition by beta-scission ************
C6H5CH2O=R1H+C6H5CHO                        2.0E13   0.0   27.5E3 !
<estimated(j)>! INHIBE
C6H5CH2O=C6H5#+HCHO                         2.0E13   0.0   27.5E3 !
<estimated(j)>! ACCELERE
!DH = 23.59 kcal/mol!
```

```
!(j) For these beta-scissions involving the breaking of a C-C or a C-H
bond,  A-factor !
!is an average value for beta-scissions [Heyberger] and activation
energies have been!
! estimated from thermochemistry and to obtain the best results!

!C6H5CH2O=R1H+C6H5CHO                        5.26E28   -5.081   22.25E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H6#+R5CHO                        2.37E32   -6.095   28.81E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!
!C6H5CH2O=C6H5#+HCHO                         7.21E33   -6.21    36.85E3 !
mf<Da silva-bozzelli J phys chem 25(2009)6979>!

!C6H5CH2O=R1H+C6H5CHO                        1.00e14   0.00   2.91e4    !
mf<Mehl Proc comb inst 33(2011)193>!
!C6H5CH2O=C6H5#+HCHO                         1.46e20   -2.00  3.51e4    !
mf<Mehl Proc comb inst 33(2011)193>!



!***reactions with oxygen
C6H5CH2O+O2=R3OOH+C6H5CHO                    6.0E10   0.0   1.6E3  !
<estimated(k)>!
!(k) : Rate constant taken equal to that of the similar reaction in the
case of ethoxy!
!radicals as proposed by BAULCH92!

!*******************************!
!*REACTIONS OF CRESOXY RADICALS*!
!*******************************!

!**OC6H4CH3=HOC6H4CH2           2.9E9   1.0   3.2E3   !<estimated(h')>!
!(h') : Rate constant of the isomerisation :!
!A = ekbT/h x rpd x exp ((Dnirotx3.5)/R),  Ea = 5.9 + 5 (5 membered
transition ring)!
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2             1.1E9   1.0   22.9E3  !
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by ROO.
close bde)

!**CO elimination with rearrangement
!OC6H4CH3=>R1H+C6H6#+B2CO                  7.5E11  0.0  43.8E3 !
<FRANCK94>!
OC6H4CH3=>R1H+C6H6#+B2CO                3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>R10C2H3V+C4H4+B2CO            3.0E11  0.0  43.8E3!<FRANCK94>!
!OC6H4CH3=>C2H2+iC4H5+B2CO              3.0E11  0.0  43.8E3     !
<FRANCK94>!
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO            3.0E11  0.0  43.8E3    !
<FRANCK94>!
OC6H4CH3=>C3H3+aC3H4+B2CO               1.5E11  0.0  43.8E3     !
<FRANCK94>!
```

```
!**termination reactions!
OC6H4CH3+R1H=HOC6H4CH3                1.0E14   0.0   0.0E3  !
<estimated(g)>!

!
**********************************************************************
*********!
!*
                                        *!
!*                    SECONDARY MECHANISM OF THE OXIDATION OF TOLUENE
            *!
!*
                                        *!
!
**********************************************************************
*********!

!************************************************!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!************************************************!

! Amorcage
!C6H5CHO+O2=C6H5CO+R3OOH         2.0E13   0.0   38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R3OOH          7.0E11   0.0   39.5E3 !RODA RODA
C6H5CHO = C6H5CO + R1H    3.98E15 0.0 83.74E3  !NIST GRELA86!

! Addition
C6H5CHO+R1H=C6H6#+R5CHO          5.8E13   0.0   8.1E3       !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13     0.0        3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the  resonnance
stabilisation of the!
! obtained radical!

C6H5CHO+B1O=C6H5CO+R2OH          6.0E12     0.0   1.8E3 !<BAULCH94>!
C6H5CHO+R2OH=C6H5CO+H2O          7.8E12     0.0   0.0   !<BAULCH94>!
C6H5CHO+R3OOH=C6H5CO+H2O2  3.0E12     0.0   11.0E3     !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4   2.0E-6     5.6   2.5E3 !MF <BAULCH94>!

C6H5CHO+R11C2H5=C6H5CO+C2H6      1.3E12     0.0   7.5E3 !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the  !
!resonnance stabilisation of the obtained radical!
```

```
C6H5CHO+C3H5Y=C6H5CO+C3H6Y 1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2     1.3E12         0.0          11.5E3      !
<estimated(p)>!
C6H5CHO+nC4H5=C6H5CO+C4H6Z2     1.3E12         0.0           7.5E3      !
<estimated(p)>!
C6H5CHO+benzyl=toluene+C6H5CO         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5O#=C6H5CO+C6H5OH#         1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+OC6H4CH3=C6H5CO+HOC6H4CH3     1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C5H5#=C6H5CO+C5H6#      1.3E11     0.0   11.5E3     !
<estimated(p)>
!(p) :Rate constant taken equal to that of the H-abstraction with ethyl
radicals  !
! with A divided by 10 for cyclic radicals and with an activation
energy !
!4 kcal/mol higher for resonnance stabilised radicals!

C6H5CHO+HOC6H4CH2=C6H5CO+HOC6H4CH3    1.3E11     0.0   11.5E3     !
<estimated(p)>
C6H5CHO+C6H5#=C6H5CO+C6H6#      1.3E11     0.0   11.5E3   !<estimated(p)>

C6H5CO=C6H5#+B2CO                       4E14   0.0      29.5e3   !
<SOLLY71>!
!Author(s):   Solly, R.K.; Benson, S.W.
!Title:   Kinetics of the gas-phase unimolecular decomposition of the
benzoyl radical
!Journal:   J. Am. Chem. Soc.
!Volume:   93
!Page(s):   2127
!Year:   1971

!************************************!
!*REACTIONS OF BENZYL HYDROPEROXYDE*!
!************************************!

!MFC6H5CH2OOH=C6H5CH2O+R2OH           1.5E16     0.0   42.0E3     !
<estimated(r)>!
!(r) : Rate constant taken equal to that the decomposition of
hydroperoxide species !
! proposed by Bounaceur <SAHETCHIAN>!
!MFC6H5CH2OOH=C6H5CH2O+R2OH           2.03E47         -10.27
     50.71E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OOH=C6H5CH2O+R2OH         3.29E13         0.42       39.89E3  !
MF<da silva Proc comb inst 32(2009)287-294>
C6H5CH2OOH=C6H5CHO+H2O                7.45E8          1.19
     46.04E3  !MF<da silva Proc comb inst 32(2009)287-294>


!****************************************!
!*REACTIONS OF CRESOL AND DERIVED RADICALS*!
!****************************************!
```

```
! amorcage
HOC6H4CH3+O2=OC6H4CH3+R3OOH          1.0E13     0.0   38.9E3     !
<estimated(s)>! ralenti
!A=1E13 pour phenol!
!(s) : Rate constant taken equal to that of the same reaction for
phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R3OOH        2.1E13      0.0       38.0E3    !
<EMDEE92*2>!
HOC6H4CH3+O2=HOC6H4CH2+R3OOH         2.1E12      0.0       38.6E3    !
RODA <estimated(aaa)>!

! addition
HOC6H4CH3+R1H=C6H5OH#+R4CH3             5.8E13      0.0          8.1E3
!<estimated(t)>!
!(t) : Rate constant taken equal to that of the same reaction for toluene
!

!HOC6H4CH2+B1O=C6H4OH#+HCHO 8E13 0.0 0.0




! metatheses
HOC6H4CH3+R1H=OC6H4CH3+H2          1.2E14  0.0   12.4E3     !
<estimated(s)>!
HOC6H4CH3+B1O=OC6H4CH3+R2OH             1.3E13  0.0   2.9E3 !
<estimated(s)>!
HOC6H4CH3+R2OH=OC6H4CH3+H2O           1.4E8 1.4   -0.96E3    !
<estimated(s)>!
HOC6H4CH3+R3OOH=OC6H4CH3+H2O2         1.0E12     0.0   10.0E3     !
<estimated(s)>!
HOC6H4CH3+R4CH3=OC6H4CH3+CH4          1.8E11     0.0   7.7E3 !
<estimated(s)>!
HOC6H4CH3+C6H5#=OC6H4CH3+C6H6#        4.9E12     0.0   4.4E3 !
<estimated(s)>!
HOC6H4CH3+C5H5#=OC6H4CH3+C5H6#        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y        4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2       4.9E11     0.0   9.4E3   !
<estimated(s)>!
HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH#     4.9E11     0.0   9.4E3   !
<estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2          1.2E14      0.0       8.4E3   !
<estimated(t)>!
HOC6H4CH3+B1O=HOC6H4CH2+R2OH          6.3E11         0.0
0.0     !<estimated(t)>!
HOC6H4CH3+R2OH=HOC6H4CH2+H2O          5.2E9       1.0       0.87E3  !
<estimated(t)>!
```

```
HOC6H4CH3+R3OOH=HOC6H4CH2+H2O2        4.0E11      0.0       14.0E3  !
<estimated(t)>!
HOC6H4CH3+R4CH3=HOC6H4CH2+CH4         1.6E12         0.0       11.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H5Y=HOC6H4CH2+C3H6Y 1.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C3H3=HOC6H4CH2+pC3H4        1.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+iC4H5=HOC6H4CH2+C4H6Z21.6E12         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+nC4H5=HOC6H4CH2+C4H6Z2      1.6E12         0.0       11.1E3  !
<estimated(t)>!
HOC6H4CH3+C5H5#=HOC6H4CH2+C5H6# 1.6E11         0.0       15.1E3  !
<estimated(t)>!
HOC6H4CH3+C6H5#=HOC6H4CH2+C6H6# 7.9E13      0.0       12.0E3    !
<estimated(t)>!
HOC6H4CH3+C6H5O#=HOC6H4CH2+C6H5OH#    1.6E11         0.0       15.1E3   !
<estimated(t)>!
HOC6H4CH3+C6H4CH3=HOC6H4CH2+toluene   7.9E13      0.0       12.0E3   !
<estimated(t)>!
HOC6H4CH3+OC6H4CH3=HOC6H4CH2+HOC6H4CH3          1.6E11     0.0
15.1E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2OO=HOC6H4CH2+C6H5CH2OOH   4.0E11     0.0
14.0E3   !<estimated(t)>!
HOC6H4CH3+C6H5CH2O=HOC6H4CH2+C6H5CH2OH          1.6E11     0.0
11.1E3   !<estimated(t)>!

HOC6H4CH2+O2=HOC6H4CH2OO              4.6E11     0.0   -377.0     !
<estimated(u)>!
HOC6H4CH2+O2=HOC6H4CH2O+B1O           6.3E12     0.0   40.0E3     !
<estimated(u)>!
HOC6H4CH2+R3OOH=HOC6H4CH2O+R2OH       5.0E12     0.0   0.0   !
<estimated(u)>!
!(u) : Rate constant taken equal to that of the same reaction for benzyl
radicals !

HOC6H4CH2+R1H=HOC6H4CH3               1.0E14     0.0   0.0   !
<estimated(g)>!
HOC6H4CH2+R4CH3=C6H5OH#+C2H4Z         5.0E12     0.0   0.0   !
<estimated(g)>!

HOC6H4CH2OO=C6H4OHCHO+R2OH      3.4E9 1.0   37.5E3     !<estimated(v)>!
!(v) : Rate constant taken equal to that of the same reaction for benzyl
peroxy radicals !

HOC6H4CH2O=R1H+C6H4OHCHO              2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O=C6H4OH#+HCHO               2.0E13     0.0       27.5E3     !
<estimated(w)>!
HOC6H4CH2O+O2=R3OOH+C6H4OHCHO         6.0E10      0.0       1.6E3     !
<estimated(w)>!
!(w) : Rate constant taken equal to that of the same reaction for benzyl
alcoxy radicals !
```

```
C6H4OHCHO+R1H=C6H4OHCO+H2       4.0E13     0.0   3.2E3 !<estimated(x)>!
C6H4OHCHO+B1O=C6H4OHCO+R2OH           6.0E12     0.0   1.8E3 !
<estimated(x)>!
C6H4OHCHO+R2OH=C6H4OHCO+H2O           7.8E12     0.0   0.0   !
<estimated(x)>!
C6H4OHCHO+R3OOH=C6H4OHCO+H2O2         3.0E12     0.0   11.0E3     !
<estimated(x)>!
C6H4OHCHO+R4CH3=C6H4OHCO+CH4          2.0E-6     5.6   1.5E3 !
<estimated(x)>!
!(x) : Rate constant taken equal to that of the same reaction for
benzaldehyde !

C6H4OHCO=C6H4OH#+B2CO               2.0E13 0.0   30.5E3     !
<estimated(y)>
!(y) : Rate constant taken equal to that of the same reaction for C6H5CO
radicals !

!************************************************!
!*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS*!
!************************************************!

C6H5CH2OH+O2=R3OOH+C6H5CHOH           1.4E12     0.0   34.0E3    !RODA
<estimated(aaa)>!
C6H5CH2OH+O2=C6H5CH2O+R3OOH           2.0E14     0.0   41.4E3    !
<EMDEE92>!

C6H5CH2OH+R1H=C6H6#+R6CH2OH           5.8E13  0.0     8.1E3     !
<estimated(t)>!

C6H5CH2OH+R1H=C6H5CHOH+H2       8.0E13     0.0   6.4E3 !<estimated(t')>!
C6H5CH2OH+B1O=C6H5CHOH+R2OH           4.2E11     0.0    -2.0E3   !
<estimated(t')>!
C6H5CH2OH+R2OH=C6H5CHOH+H2O           3.5E9 1.0    -1.13E3  !
<estimated(t')>!
C6H5CH2OH+R3OOH=C6H5CHOH+H2O2         2.7E11     0.0   12.0E3     !
<estimated(t')>!
C6H5CH2OH+R4CH3=C6H5CHOH+CH4          1.1E12     0.0   9.1E3 !
<estimated(t')>!
C6H5CH2OH+C3H5Y=C6H5CHOH+C3H6Y          1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+iC4H5=C6H5CHOH+C4H6Z2         1.1E12   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+nC4H5=C6H5CHOH+C4H6Z2         1.112    0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C6H5#=C6H5CHOH+C6H6#        5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H4CH3=C6H5CHOH+toluene    5.2E13     0.0   10.0E3     !
<estimated(t')>!
C6H5CH2OH+C6H5O#=C6H5CHOH+C6H5OH#       1.1E11   0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+benzyl=C6H5CHOH+toluene     1.1E11     0.0   13.1E3     !
<estimated(t')>!
C6H5CH2OH+OC6H4CH3=C6H5CHOH+HOC6H4CH3 1.1E11     0.0   13.1E3     !
<estimated(t')>!
```

```
C6H5CH2OH+HOC6H4CH2=C6H5CHOH+HOC6H4CH3     1.1E11     0.0   13.1E3  !
<estimated(t')>!
C6H5CH2OH+C5H5#=C6H5CHOH+C5H6#        1.1E11     0.0   13.1E3  !
<estimated(t')>!
!t': estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H                    2.0E13     0.     36.373E3    !MF
DHr=36.79 correlation baptiste E=0.6*DHr+14.3
!R15C2H5O=CH3CHO+R1H                2.0E14     0.     23.3E3 !(243,-
243)<HEICKLEN88NIST>!


!***********************************************!
!*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS*!
!***********************************************!

!** Amorзages monomolйculaires
etC6H5 = R1H + C8H9#     4.3E14 0.0 83.6E3   !<kingas>!

!** Amorзages bimolйculaires
etC6H5+O2=C8H9#+R3OOH             1.4E12   0.0   34.0E3    !
<estimated(aaa)>!
etC6H5+O2=C8H9#-1+R3OOH           1.2E13        0.0     49.0E3    !
<exgas>!

!** Additions ipso
etC6H5+R1H=C6H6#+R11C2H5           5.8E13       0.0   8.1E3    !
<estimated(t)>!

!** Metatheses
etC6H5+R1H=C8H9#+H2                   8.0E13     0.0        6.4E3
     !<estimated(t")>!
etC6H5+B1O=C8H9#+R2OH            4.2E11     0.0    -2.0                !
<estimated(t")>!
etC6H5+R2OH=C8H9#+H2O            3.5E9 1.0    -1.13E3        !
<estimated(t")>!
etC6H5+R3OOH=C8H9#+H2O2               2.7E11     0.0        12.0E3
     !<estimated(t")>!
etC6H5+R4CH3=C8H9#+CH4              1.1E12  0.0        9.1E3           !
<estimated(t")>!
etC6H5+C3H5Y=C8H9#+C3H6Y         1.1E12     0.0        13.1E3          !
<estimated(t")>!
etC6H5+iC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+nC4H5=C8H9#+C4H6Z2      1.1E12 0.0        13.1E3          !
<estimated(t")>!
etC6H5+C6H5O#=C8H9#+C6H5OH#     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+benzyl=C8H9#+toluene     1.1E11     0.0        13.1E3          !
<estimated(t")>!
etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11     0.0        13.1E3             !
<estimated(t")>!
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```
etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11    0.0        13.1E3          !
<estimated(t")>!
etC6H5+C5H5#=C8H9#+C5H6#        1.1E11     0.0        13.1E3          !
<estimated(t")>!

!t": estimated as toluene with A x(2/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2      7.2E8      1.5        6.79E3     !MF
correlation Dean-Bozzelli 2000
etC6H5+B1O=C8H9#-1+R2OH         5.1E8      1.5        5.05E3          !MF
correlation Dean-Bozzelli 2000
etC6H5+R2OH=C8H9#-1+H2O         3.6E6      2.0        4.82E2     !MF
correlation Dean-Bozzelli 2000
etC6H5+R3OOH=C8H9#-1+H2O2  4.2E4      2.69  1.85E4           !MF
correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4   2.43E6     1.87  1.03E4     !MF correlation
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9#        5.27E13   0.0    12.0E3  !ajout MF as
2/3 toluene <HECKMANN96>!
etC6H5+C6H5#=C6H6#+C8H9#      5.27E13   0.0    9.0E3   !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1    5.85E10   0.0    3.83E3  !ajout MF as
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>


! Ajout ipso MF
etC6H5+B1O=C6H5O#+R11C2H5  1.7E13   0.0     3.6E3    !MF as toluene !
<TAPPE89>!
etC6H5+R2OH=C6H5OH#+R11C2H5  1.3E13   0.0    10.6E3    !MF as toluene
<BAULCH94>as benzene
!etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.59E4    !MF as benzene
<Robaugh,J. Phys. Chem.90(1986)4159 - 4163>
etC6H5+R4CH3=toluene+R11C2H5 1.2E12   0.0    1.24E4    ! MF as benzene-
kcal <Robaugh,J. Phys. Chem.90(1986)4159 - 4163>

!** Decompositions

C8H9#-1=C2H4Z+C6H5#     2.0E13   0.0      35.5E3 !MF correlation exgas
C8H9#  =R1H+styrene        3.1e13   0.0      50670      !<MULLER88>
C8H9#-1=R1H+styrene        4.0E13   0.0      33.58E3    !MF <Sirjean,
J.Phys.Chem.A 2008>

!** Reactions of derived radicals
C8H9#+O2=R3OOH+styrene                      6.90E11          0.0
15.2E3      !<est (exgas-sylvain)>!

!C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO                   3.27E12          0.0
0.0      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R3OOH=R2OH+R1H+C6H5COCH3                   7.80E10          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
```

```
!C8H9#+R3OOH=>R2OH+C6H5#+CH3CHO                    2.54E11          0.0
0.0         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R3OOH=C8H9#OOH                               3.60E12          0.0
0.0    !MF KINGAS
C8H9#OOH=R2OH+C8H9#O                               5.00E15
0.0     42500          !MF
C8H9#O=R4CH3+C6H5CHO                               2.69E13          0.0
12117      !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
C8H9#O=C6H5#+CH3CHO                                    1.74E14
0.0      20458         !MF  as but-3-en-1-oxy <Rauk, Can.J.Chem
81(2003)431-442>

C8H9#-1+O2=R3OOH+styrene                       2.60E11          0.0
2.5E3
C8H9#-1+R3OOH=R2OH+HCHO+benzyl                 5.00E12          0.0
0.0      !<kingas>!

!*****************************************!
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!
!*****************************************!

styrene+O2=R3OOH+C6H5C2H2          2.0E13       0.0        57.9E3  !
<asbutadiene/2>!
!C4H6Z2+O2=iC4H5+R3OOH             4.0E13       0.0        57.9E3  !
<LEUNG95>!


!styrene+B1O=C6H5#+R13CH2CHO        3.0E08       1.45        0.9E3  !
<asbutadiene/2>! ! ENLEVE PAR BENOIT ET PAG
styrene+R2OH=benzyl+HCHO           1.4E12       0.0        -0.9E3  !<as
butadiene/2!
styrene+R2OH=C6H5CHO+R4CH3         1.4E12       0.0        -0.9E3  !MF
idem rйaction prйcйdente as C3H6Y <TSAnG91>

!C4H6Z2+B1O=C3H5Y+R1H+B2CO         6.0E08       1.45        0.9E3  !
<LEUNG95,BREZINSKY84>!
!C4H6Z2+R2OH=C3H5Y+HCHO            2.8E12       0.0        -0.9E3  !
<LINSTEDT96>!
!C4H6Z2+R2OH=CH3CHO+R10C2H3V       5.6E12       0.0        -0.9E3  !
<fromLINSTEDT96>!

styrene+R1H=C6H5C2H2+H2            3.3E5        2.53        9.2E3  !MF<as
butadiene/2>!
styrene+R2OH=C6H5C2H2+H2O          1.5E6        2.0         0.4E3  !<as
butadiene/2>!
styrene+R4CH3=C6H5C2H2+CH4        3.5E13       0.0        15.5E3  !<as
butadiene/2>


!C4H6Z2+R1H=iC4H5+H2               6.6E5        2.53        9.2E3  !
<WANG97>!
!C4H6Z2+R2OH=iC4H5+H2O             3.1E6        2.0         0.4E3  !
<WANG97>!
```

```
!C4H6Z2+R4CH3=iC4H5+CH4            7.0E13       0.0        15.5E3  !
<WU87-3kcal>!

C6H5C2H2+O2=C6H5CO+HCHO            4.5E16      -1.39        1.0E3  !
<asMebel C2H3+O2>! **


!*Addition Zhenyu*!
C6H5C2H2+R1H=C6H5#C2H+H2                1.0E13       0.0
0.0  !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and
Tech. 120 (1996) 119-167.
C6H5C2H2+R2OH=C6H5#C2H+H2O         1.0E13       0.0           0.0  !in
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120
(1996) 119-167.

! ajout d'un amorcage Roda
C6H5#C2H   => C6H5# + R9C2H     2.2e16          0.0        98.0e3  ! MF
as toluene



!*****************************************!
!*REACTIONS OF C5H5CCH AND DERIVED RADICALS *!
!*****************************************!

!*Addition Zhenyu*!
!C5H5CCH=C5H5#+R9C2H                      4.2E15     0.0   125.0E3    !
<KInGAS1500>! pC3H4=R9C2H+R4CH3
!C5H5CCH+R1H=C5H5#+C2H2                  2.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R1H=C3H3+C4H4                   6.0E10     0.0             0.0
     !Lindstedt96
!C5H5CCH+R2OH=C5H5#+CH2COZ               4.3E11     0.0         -0.8E3
     !<BOODAGHIAnS87>!pC3H4+R2OH=CH2COZ+R4CH3
!C5H4CCH2=C5H5CCH                     2.5E12     0.0    59.0E3    !
<HIDAKA89>!aC3H4=pC3H4
!C5H4CCH2+R1H=C5H5CCH+R1H             8.5E12     0.0     2.0E3    !
<WAGnER72>!aC3H4+R1H(+M)=tC3H5(+M)
!C5H4CCH2+R2OH=C5H5#+CH2COZ           2.0E12     0.0      -0.2E3 !<LIU88>!
aC3H4+R2OH=CH2COZ+R4CH3

!*****************************************!
!*REACTIONS OF BIBENZYL AND DERIVED RADICALS*!
!*****************************************!

bibenzyl=C14H13#+R1H                  1.0E16      0.0    83.66E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
bibenzyl+O2=C14H13#+R3OOH              2.8E12      0.0     35.0E3   !<est
aaaa!
bibenzyl+R1H=C14H13#+H2                   5.4E4       2.5     -1.9E3   !
Table A-I-21 Zhenyu

bibenzyl+B1O=C14H13#+R2OH              8.4E11      0.0       -2.0   !
<estimated(t"')>!
```

```
bibenzyl+R2OH=C14H13#+H2O              7.0E9           1.0    -1.13E3   !
<estimated(t"')>!

bibenzyl+R3OOH=C14H13#+H2O2           5.4E11      0.0   12.0E3   !
<estimated(t"')>!
bibenzyl+R4CH3=C14H13#+CH4            2.2E12      0.0      9.1E3   !
<estimated(t"')>!
bibenzyl+C6H5O#=C14H13#+C6H5OH#        2.2E12      0.0     13.1e3   !
<estimated(t"')>!
bibenzyl+benzyl=C14H13#+toluene       2.2E12      0.0    9.1E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu

bibenzyl+C3H5Y=C14H13#+C3H6Y          2.2E12      0.0   13.1E3   !
<estimated(t"')>!
!t"': estimated as toluene with A x(4/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF
bibenzyl+R1H=C6H6#+C8H9#-1        5.67E8   1.43   5.65E3    !Calcul CBS-
QB3 Fournet as toluene
bibenzyl+R2OH=C6H5OH#+C8H9#-1      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006
C14H13#=stilbene+R1H               7.94E15  0.0   51.864E3   !
<Oehlschlaeger05>! in Sakai07 Zhenyu
C14H13#+O2= stilbene+R3OOH         1.6E12  0.00  15200  !as allylique
C14H13#+R3OOH=>R2OH+C6H5CHO+benzyl  8.21E4   2.20  -5.13E3 ! as benzyl

!*******************************************!
!*REACTIONS OF STILBENE                     *!
!*******************************************!
!Ajout Ipso MF
stilbene+R1H=>C6H6#+C2H2+C6H5#      5.67E8   1.43   5.65E3  !Calcul CBS-
QB3 Fournet as toluene
stilbene+R2OH=C6H5OH#+C6H5C2H2      7.83E2   2.884  3.2193E3  !Seta V
Nakajima V Miyoshi JPCA 2006

! ajout MF
stilbene+R2OH=C6H5CHO+benzyl       1.0E13       0.0        5.94E3  !
<Baulch05> as C2H4

!*************************************************!
!* Reactions of naphthalene                      *!
!*************************************************!
2C5H5#=naphthalene+H2           4.3E36  -6.3  22.835E3 ! A.M. Dean, J.
Phys. Chem. 94 (1990) 1432-1439.
C6H5#+iC4H3=naphthalene         3.18E23 -3.2  2.13E3   ! H.Y. Zhang, J.T.
McKinnon, CST 107 (1995) 261-300.
C6H5#+C4H4=naphthalene+R1H      3.3E33  -5.7  12.75E3  ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
benzyl+C3H3=>naphthalene+R1H+R1H 6.0E11  0.0  0.0      ! M.B. Colket,
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
C6H5C2H2+C2H2=naphthalene+R1H   1.6E16  -1.33 3.3E3    ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
```

```
naphthalene+O2=R3OOH+naphthyl          8.0E13      0.0        63.4E3   !
like benzene <ALZUETA00>A*8/6!
naphthalene+B1O=>indenyl+B2CO+R1H      2.7E13      0.0      3.6E3   !like
benzene <Nicovich82>A*8/6!
naphthalene+R1H=naphthyl+H2            8.0E8       1.8     16.8E3  !like
benzene <MEBEL97>A*8/6!
naphthalene+B1O=naphthyl+R2OH          2.7E13      0.0     14.7E3  !like
benzene <LINDSTEDT94>A*8/6!
naphthalene+R2OH=naphthyl+H2O          2.1E8       1.42    1.45E3  !like
benzene <BAULCH92>A*8/6!
naphthalene+R3OOH=naphthyl+H2O2        7.3E12      0.0     28.9E3  !like
benzene <BAULCH94>A*8/6!
naphthalene+R4CH3=naphthyl+CH4         2.7E12      0.0     15.0E3  !like
benzene <ZHANG89>A*8/6!

naphthyl+R1H=naphthalene          1.0E14   0.0   0.0E3  !as n-
buthylbenzene
naphthyl+O2=>indenyl+B2CO+B1O     2.6E13   0.0   6.1E3  !as n-
buthylbenzene
naphthyl+B1O=>indenyl+B2CO        1.0E14   0.0   0.0    !as n-
buthylbenzene
naphthyl+R3OOH=>indenyl+B2CO+R2OH 5.0E12   0.0   0.0    !as n-
buthylbenzene
naphthyl+R2OH=>indenyl+B2CO+R1H   1.0E13   0.0   0.0    !as n-
buthylbenzene

!************************************************!
!* Reactions of indene and derived radicals       *!
!  Indene C6H4#/CH2/CH//CH/                      *!
!  Indenyl C6H4#/CH/CH//CH/                      *!
!  ph#C3H2  C6H5#/CH(.)/C///CH                   *!
!************************************************!

indene+R2OH=>C2H4Z+C6H5CO             1.37E12  0.0  -1.04E3  !Slavinskaya
indene+R2OH=>R10C2H3V+B2CO+C6H6#      1.37E12  0.0  -1.04E3 !Est.
!indene+R2OH=>o-methylbenzyl+B2CO     1.37E12  0.0  -1.04E3

indene+O2=R3OOH+indenyl               1.4E12   0.0   31.03E3  ! as n-
buthylbenzene mais E = DH de reaction
indene+B1O=indenyl+R2OH               1.76E11  0.7   3.25E3  ! A-I-21
secondary  A*2
indene+R1H=indenyl+H2                 1.08E5   2.5   -1.9E3  ! A-I-21
secondary  A*2
indene+R2OH=indenyl+H2O               6.0E6    2.0   -1.52E3 ! A-I-21
secondary  A*2
indene+R4CH3=indenyl+CH4              2.0E11   0.0   7.3E3   ! A-I-21
secondary  A*2
indene+R3OOH=H2O2+indenyl             1.28E4   2.6   12.4E3  ! A-I-21
secondary  A*2

!indene+R1H=ph#C3H4Y         5.8E13  0.0  8.1E3  !ipso-addition
!indene+R1H=ph#C3H4-1        5.8E13  0.0  8.1E3  !ipso-addition
```

```
indene+R1H=>C2H2+benzyl       1.16E14  0.0  8.1E3 !mf 2x ipso-addition

indenyl=>C5H5#+C4H2           5.0E13   0.0  75.0E3  !Slavinskaya09
5.0E13  0.0  37.5E3
indenyl+R1H=indene           1.0E14   0.0   0.0    !as n-buthylbenzene
C6H5#+C3H3=indene            6.46E12  0.0   0.0    !Slavinskaya09
!indenyl+R3OOH=>C6H6#+B2CO+R9C2H+R2OH    3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2
indenyl+R3OOH=>C6H5#C2H+R5CHO+R2OH         3.0E12   0.0   0.0    ! Est.!
similar to C5H5#+HO2

indenyl+B1O=>C6H6#+B2CO+R9C2H          5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H
indenyl+B1O=>C6H5#C2H+R5CHO           5.8E13  -0.02  0.02E3 !Est.
C5H5#+B1O=C5H4O#+R1H

indenyl+R2OH=>styrene+B2CO   4.0E14   0.0   4.5E3  !Est.
C5H5#+OH=C4H6Z2+CO

!C9H7O#=C9H6O#+R1H          2.0E13  0.0  27.5E3   ! Est.like ph#CH2O
!C9H7O#=>C6H6#+B2CO+R9C2H   2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO
!C9H7O#=C6H5#C2H+R5CHO      2.8E13  0.0  17.1E3   ! Est.CH3CO=CH3+CO
!
!*************************************************************************
*********************************
!*************************************Reactions for Ethyl
Esters*****************************************
!
!*************************************************************************
*********************************
EF=HCOOH+C2H4Z                       2.000E+12   0.00  4.729E+04
!EF(+m)=HCOOH+C2H4Z(+m)               4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
C2H5OCO+R1H(+m)=EF(+m)               1.000E+14   0.00  0.000E+00
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /
TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off
reaction
EFEJ+R1H(+m)=EF(+m)                  1.000E+14   0.00  0.000E+00
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off
reaction
EFMJ+R1H(+m)=EF(+m)                  1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EF(+m)=R5CHO+R15C2H5O(+m)             1.650E+24  -2.04  1.002E+05
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off
reaction
EF(+m)=HCO2+R11C2H5   (+m)               5.734E+25  -2.76  9.211E+04
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /
```

```
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off
reaction
EF(+m)=CH2OCHO+R4CH3(+m)            3.388E+21  -1.58  9.209E+04
LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /
TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off
reaction
EF+O2=C2H5OCO+R3OOH               2.000E+13   0.00  4.130E+04   !as ep
-3kcal
EF+O2=EFEJ+R3OOH                  2.000E+13   0.00  4.820E+04   !as ep
EF+O2=EFMJ+R3OOH                  3.000E+13   0.00  5.229E+04   !as ep

EF+R1H=C2H5OCO+H2                   2.720e+07   1.94     7880.0   !Good
et al.
EF+R1H=EFEJ+H2                      1.790E+05   2.53  3.420E+03   !as
C2H5OH PARk et al., J.Chem.Phys. 118 (2003) 9990-9996
EF+R1H=EFMJ+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EF+B1O=C2H5OCO+R2OH                   5.510e+05   2.5   2.830e+03   !
Westbrook et al.,
EF+B1O=EFEJ+R2OH                      1.450E+05   2.47  8.800E+02   !as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703
EF+B1O=EFMJ+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EF+R2OH=C2H5OCO+H2O                 1.610e+06   1.87       30.0   !Good
et al.
EF+R2OH=EFEJ+H2O                    1.306E+05   2.43    -1457.0   ! Xu
Lin pci 2007 31 159-166
EF+R2OH=EFMJ+H2O                    5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EF+R4CH3=C2H5OCO+CH4                6.564e+01   3.32    10010.0   !Good
et al.
EF+R4CH3=EFEJ+CH4                   1.990E+01   3.37     7635.0   !
Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
EF+R4CH3=EFMJ+CH4                   4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EF+R3OOH=C2H5OCO+H2O2               9.640e+03   2.6   1.391e+04   !
Westbrook et al.,
!EF+R3OOH=EFEJ+H2O2                  8.200E+03   2.55    10750.0   !
MARinov 1998
EF+R3OOH=EFEJ+H2O2                  3.610E+03   2.55  1.053E+04
EF+R3OOH=EFMJ+H2O2                  8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EF+R8CH3OO=C2H5OCO+CH3OOH           4.820E+03   2.6   1.391E+04   !
Westbrook et al.,
EF+R8CH3OO=EFEJ+CH3OOH              7.220E+03   2.55  1.053E+04
EF+R8CH3OO=EFMJ+CH3OOH              8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EF+R7CH3O  =C2H5OCO+CH3OH             1.620e+12   0.00     8190.0   !
Herron
EF+R7CH3O  =EFEJ+CH3OH                4.580E+10   0.00  2.873E+03
EF+R7CH3O  =EFMJ+CH3OH                1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
```

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!EFEJ+O2=EFeoo                      1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EFMJ+O2=EFmoo                      9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!EFeoo=EFED+R3OOH                   5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EFmoo=EFED+R3OOH                   5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal

C2H5OCO=R15C2H5O+B2CO                4.840E+10    1.11    15887.0 !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
                          rev / 3.570E+04    2.485   37247.0 /
C2H5OCO=R11C2H5   +CO2                8.020E+11    0.65    21123.0 !
Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
                          rev / 1.350E+04    2.31     7883.0 /
EFEJ=CH3CHO+R5CHO                   1.127E+21  -1.73  4.055E+04
EFMJ=C2H4Z+HCO2                      1.340E+13  -0.40  2.461E+04  !
Westbrook et al., (2009)

EFEJ=EFED+R1H                         3.000e+13   0.00  3.900e+04  !ST
EFMJ=EFED+R1H                         3.000e+13   0.00  3.800e+04  !ST

!EFEJ+O2=EFED+R3OOH                  1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EFMJ+O2=EFED+R3OOH                  1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
EFEJ+R3OOH=EFED+H2O2                  2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
EFMJ+R3OOH=EFED+H2O2                  2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)

HCHO+R2OH=HCOOH+R1H                    4.450E+07    1.18     -447.0   !
(TSANG HAMPSON 86)
HCOOH+M=B2CO+H2O+M                   2.300E+13    0.0     50000.0   !
(82HSU/SHA)
HCOOH+M=CO2+H2+M                  1.500E+16    0.0     57000.0   !
(82HSU/SHA)
HCOOH+R2OH=HCO2+H2O                   2.710E+11    0.0         0.0   !
(92ATK/BAU)
HCO2=>R1H+CO2                         1.740E+12    0.31    32928.0   !
(88LAR/STE)
EFED+R2OH=>HCHO+CH2OCHO               1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EFED+R2OH=>CH3CHO+HCO2                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802

EA=CH3COOH+C2H4Z                     2.000E+12   0.00  4.729E+04
!EA(+m)=CH3COOH+C2H4Z(+m)             4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
EA2J+R1H(+m)=EA(+m)                   1.000E+14   0.00  0.000E+00
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /
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TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off
reaction
EAEJ+R1H(+m)=EA(+m)                 1.000E+14   0.00  0.000E+00
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off
reaction
EAMJ+R1H(+m)=EA(+m)                 1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EA(+m)=C2H5OCO+R4CH3(+m)            2.627E+27  -3.23  9.769E+04 !as ep
+3kcal
LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /
TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off
reaction
EA(+m)=R14CH3CO+R15C2H5O(+m)          1.650E+24  -2.04  1.002E+05
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off
reaction
EA(+m)=CH3CO2+R11C2H5   (+m)            5.734E+25  -2.76  9.211E+04
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off
reaction
EA(+m)=MEMJ+R4CH3(+m)               3.388E+21  -1.58  9.209E+04
LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /
TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off
reaction
EA+O2=EA2J+R3OOH                  2.000E+13   0.00  4.730E+04   !as ep
+3kcal
EA+O2=EAEJ+R3OOH                  2.000E+13   0.00  4.820E+04   !as ep
EA+O2=EAMJ+R3OOH                  3.000E+13   0.00  5.229E+04   !as ep

EA+R1H=EA2J+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EA+R1H=EAEJ+H2                      1.790E+05   2.53  3.420E+03   !as
C2H5OH PARk et al., J.Chem.Phys. 118 (2003) 9990-9996
EA+R1H=EAMJ+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
!EA+R1H=EAMJ+H2                     6.660E+05   2.54  6.756E+03
EA+B1O=EA2J+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EA+B1O=EAEJ+R2OH                      1.450E+05   2.47  8.800E+02   !as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703
EA+B1O=EAMJ+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
!EA+B1O=EAMJ+R2OH                     9.810E+05   2.43  4.750E+03
EA+R2OH=EA2J+H2O                    5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EA+R2OH=EAEJ+H2O                    1.306E+05   2.43    -1457.0   !as
C2H5OH Xu Lin pci 2007 31 159-166
EA+R2OH=EAMJ+H2O                    5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
!EA+R2OH=EAMJ+H2O                    5.280E+09   0.97  1.586E+03
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EA+R4CH3=EA2J+CH4                    4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EA+R4CH3=EAEJ+CH4                    1.990E+01   3.37     7635.0   !as
C2H5OH Xu et al., J.Chem.Phys. 120, 6593-6599 (2004)
EA+R4CH3=EAMJ+CH4                    4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
!EA+R4CH3=EAMJ+CH4                    4.530E-01   3.65  7.154E+03
EA+R3OOH=EA2J+H2O2                   8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
!EA+R3OOH=EAEJ+H2O2                   8.200E+03   2.55    10750.0   !
MARinov 1998
EA+R3OOH=EAEJ+H2O2                   3.610E+03   2.55  1.053E+04
EA+R3OOH=EAMJ+H2O2                   8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
!EA+R3OOH=EAMJ+H2O2                   2.379E+04   2.55  1.649E+04
EA+R8CH3OO=EA2J+CH3OOH               8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EA+R8CH3OO=EAEJ+CH3OOH               7.220E+03   2.55  1.053E+04
EA+R8CH3OO=EAMJ+CH3OOH               8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
!EA+R8CH3OO=EAMJ+CH3OOH               2.379E+04   2.55  1.649E+04
EA+R7CH3O  =EA2J+CH3OH                1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
EA+R7CH3O  =EAEJ+CH3OH                4.580E+10   0.00  2.873E+03
EA+R7CH3O  =EAMJ+CH3OH                1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
!EA+R7CH3O  =EAMJ+CH3OH                2.169E+11   0.00  6.458E+03

!EAMJ=EA2J                           9.900E+07   1.00   12000.0  ! IS 26 KB
!EAEJ=EA2J                           5.700E+08   1.00   21300.0  ! IS 28 KB
EA2J=EAMJ                           1.481e+08   1.00  2.450e+04   !(cyc
lact sat a 6 + 3Hp)
EA2J=EAEJ                           5.746e+08   1.00  1.800e+04   !(cyc
lact sat a 5 + 2Hs - 2kcal/O)

!!EA2J+O2=EA2oo                       9.000e+18  -2.50  0.000e+00   !Buda
et al., Combust Flame, 142 (2005) 170-186 (ks)
!EA2J+O2=EA2oo                       1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EAEJ+O2=EAeoo                       1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (all)
!EAMJ+O2=eamoo                       9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!
!eaeoo=EAED+R3OOH                    5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!eamoo=EAED+R3OOH                    5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal

!EA2J=CH2COZ  +R15C2H5O                1.280E+12   0.6584  49255.0   !
Huynh and Violi J.Org.Chem. 73 (2008) 94-101
EA2J=CH2COZ  +R15C2H5O                1.460E+12   0.61    53276.0   !
Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EA2J=CH2COZ  +R15C2H5O                9.364E+19  -1.88  5.642E+04
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!EAEJ=CH3CHO+R14CH3CO                 1.127E+21  -1.73  4.055E+04
EAEJ=CH3CHO+R14CH3CO                  1.127E+21  -1.73  4.255E+04   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EAMJ=C2H4Z+CH3CO2                   2.325E+14  -0.20  3.297E+04
EAMJ=C2H4Z+CH3CO2                    1.340E+13  -0.40  2.461E+04  !
Westbrook et al., (2009)
!EA2J*o=>C2H5OCO+B2CO                 1.834e+15  -0.73  1.291e+04   !
Glaude et al., DMC C2H5CO

EAEJ=EAED+R1H                         3.000e+13   0.00  3.900e+04  !ST
EAMJ=EAED+R1H                         3.000e+13   0.00  3.800e+04  !ST

!EAEJ+O2=EAED+R3OOH                   1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EAMJ+O2=EAED+R3OOH                   1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EAEJ+R3OOH=EAED+H2O2                  2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EAMJ+R3OOH=EAED+H2O2                  2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)

!eaeoo=eaeooH2j                       1.696e+07   1.00  2.270e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs - 2kcal/O)
!eaeooH2j+O2=eaeooH2Oo                1.700e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!eaeooH2Oo=>ea2oohe*o+R2OH             8.480e+06   1.00  2.350e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht -
2kcal/O)
!ea2oohe*o=>HCHO+B2CO+CH3CO2+R2OH      1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!eaeooH2j=>eacy2oe+R2OH               3.630e+10   0.00  1.300e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)

CH3COOH=CH2COZ  +H2O                  4.470E+14   0.00  7.989E+04   !Duan
et Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
CH3COOH=CH4+CO2                     7.080E+13   0.00  7.452E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
CH3COOH=>R14CH3CO+R2OH                 1.4E+0017   0.000  105815.7  ! UI
8 KB
CH3COOH=>CH3CO2+R1H                   2.3E+0014   0.000  106345.3  ! UI 9
KB
CH3COOH=>R4CH3+HOCO                   8.2E+0016   0.000   88817.0  ! UI 10
KB

CH3COOH+R1H=CH2COOH+H2                9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
!CH3COOH+R1H=CH3CO2+H2                 4.200E+06   2.00     2400.0   ! ME
96 CN
CH3COOH+R1H=CH3CO2+H2                 5.550E-23   10.60   -4459.0   !
PARk,Zhu,Lin, JcP 118, 9990-9996 (2003)
CH3COOH+B1O=CH2COOH+R2OH               9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
!CH3COOH+B1O=CH3CO2+R2OH                1.000E+13   0.00     3280.0   ! ME
87 CW
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CH3COOH+B1O=CH3CO2+R2OH                1.460E-03    4.73    1727.0   ! Wu,
Lee, Xu, Lin, JPcA 2007
CH3COOH+R2OH=CH2COOH+H2O             5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
!CH3COOH+R2OH=CH3CO2+H2O              1.100E+06   2.00    -1865.0   ! ME
105 CW
CH3COOH+R2OH=CH3CO2+H2O              2.810E+02    2.97    -580.0   ! Xu
Lin pci 2007 31 159-166
CH3COOH+R4CH3=CH2COOH+CH4            4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
CH3COOH+R4CH3=CH3CO2+CH4             2.035E+00    3.57    7722.0   !
Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
CH3COOH+R3OOH=>CH2COOH+H2O2          8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
!CH3COOH+R3OOH=CH3CO2+H2O2            2.110E+06   0.00  1.400E+04   ! ME
96 CN
CH3COOH+R3OOH=CH3CO2+H2O2            2.500E+12    0.00   24000.0 ! MARinov
1998
CH3COOH+R8CH3OO=CH2COOH+CH3OOH       8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
CH3COOH+R7CH3O  =CH2COOH+CH3OH         1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;

!CH2COOH=CH2COZ  +R2OH                   4.638E+18  -1.28  5.386E+04
CH2COOH=CH2COZ  +R2OH                  4.000E+13   0.00  5.821E+04
CH2COOH=>CO2+R4CH3                    1.700E+09   1.0     38640.0
!C2H5OCO=R15C2H5O+B2CO                 5.059E+14   0.17  2.552E+04
!C2H5OCO=R11C2H5   +CO2                   1.805E+16  -0.56  2.017E+04
!CH3CO2+m=R4CH3+CO2+m                 4.400E+15   0.00  1.050E+04
EAED+R2OH=>HCHO+MEMJ                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EAED+R2OH=>CH3CHO+CH3CO2             1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
HOCO=B2CO+R2OH                         1.186E+14   0.13  3.646E+04
HOCO=CO2+R1H                          8.220E+11   0.41  3.534E+04
!ea2*o+R1H=>EA2J*o+H2                  1.200E+14   0.00     7000.0   !
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!ea2*o+B1O=>EA2J*o+R2OH                5.850E+12   0.00     1808.0   !
(BAULch92)
!ea2*o+R2OH=>EA2J*o+H2O                2.650E+12   0.00     -730.0   !
Atkinson et al., 2001
!ea2*o+R3OOH=>EA2J*o+H2O2              1.700E+12    0.00   10700.0   !
(COLKET 77; CH3CHO)         3.100E+12   0.00    11920.0   !(BAULch92)

EP=C2H5COOH+C2H4Z                   2.000E+12   0.00  4.729E+04
!EP(+m)=C2H5COOH+C2H4Z(+m)            4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
EP3J+R1H(+m)=EP(+m)                   1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EP2J+R1H(+m)=EP(+m)                   1.000E+14   0.00  0.000E+00
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LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /
TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off
reaction
EPEJ+R1H(+m)=EP(+m)                 1.000E+14   0.00  0.000E+00
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off
reaction
EPMJ+R1H(+m)=EP(+m)                 1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EP(+m)=EA2J+R4CH3(+m)               5.732E+23  -2.33  8.774E+04
LOW / 4.3520E+14 8.2000E-01 6.3570E+04 /
TROE / 1.6900E-01 5.7129E+03 4.0466E+01 6.7101E+09 / !Troe Fall-off
reaction
EP(+m)=C2H5OCO+R11C2H5   (+m)           2.627E+27  -3.23  9.469E+04
LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /
TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off
reaction
EP(+m)=R25C2H5CO+R15C2H5O(+m)         1.650E+24  -2.04  1.002E+05
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off
reaction
EP(+m)=C2H5CO2+R11C2H5   (+m)           5.734E+25  -2.76  9.211E+04
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off
reaction
EP(+m)=MPMJ+R4CH3(+m)               3.388E+21  -1.58  9.209E+04
LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /
TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off
reaction
EP+O2=EP3J+R3OOH                  3.000E+13   0.00  5.229E+04
EP+O2=EP2J+R3OOH                  2.000E+13   0.00  4.430E+04
EP+O2=EPEJ+R3OOH                  2.000E+13   0.00  4.820E+04
EP+O2=EPMJ+R3OOH                  3.000E+13   0.00  5.229E+04

EP+R1H=EP3J+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
!EP+R1H=EP2J+H2                      5.400e+04   2.5  -1.900e+03   !
EP+R1H=EP2J+H2                      1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
EP+R1H=EPEJ+H2                      1.790E+05   2.53  3.420E+03   !as
C2H5OH PARk et al., J.Chem.Phys. 118 (2003) 9990-9996
EP+R1H=EPMJ+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EP+B1O=EP3J+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
!EP+B1O=EP2J+R2OH                      8.800e+10   0.70  3.250e+03   !
EP+B1O=EP2J+R2OH                      4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
EP+B1O=EPEJ+R2OH                      1.450E+05   2.47  8.800E+02   !as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703
EP+B1O=EPMJ+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
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EP+R2OH=EP3J+H2O                      5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
!EP+R2OH=EP2J+H2O                      3.000e+06   2.00 -1.520e+03   !
EP+R2OH=EP2J+H2O                      4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
EP+R2OH=EPEJ+H2O                      1.306E+05   2.43    -1457.0   !as
C2H5OH Xu Lin pci 2007 31 159-166
EP+R2OH=EPMJ+H2O                      5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EP+R4CH3=EP3J+CH4                     4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
!EP+R4CH3=EP2J+CH4                     1.000e+11   0.00  7.300e+03   !
EP+R4CH3=EP2J+CH4                     2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
EP+R4CH3=EPEJ+CH4                     1.990E+01   3.37     7635.0   !as
C2H5OH Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
EP+R4CH3=EPMJ+CH4                     4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EP+R3OOH=EP3J+H2O2                    8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
!EP+R3OOH=EP2J+H2O2                     6.400e+03   2.60  1.240e+04   !
EP+R3OOH=EP2J+H2O2                    5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!EP+R3OOH=EPEJ+H2O2                     8.200E+03   2.55    10750.0   !
MARinov 1998
EP+R3OOH=EPEJ+H2O2                    3.610E+03   2.55  1.053E+04
EP+R3OOH=EPMJ+H2O2                    8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EP+R7CH3O  =EP3J+CH3OH                  1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
!EP+R7CH3O  =EP2J+CH3OH                   1.780e+12   0.00  1.200e+03   !
EP+R7CH3O  =EP2J+CH3OH                  1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
EP+R7CH3O  =EPEJ+CH3OH                  4.580E+10   0.00  2.873E+03
EP+R7CH3O  =EPMJ+CH3OH                  1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
EP+R8CH3OO=EP3J+CH3OOH                8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EP+R8CH3OO=EP2J+CH3OOH                 6.400e+03   2.60  1.240e+04   !
EP+R8CH3OO=EP2J+CH3OOH                5.600E+12   0.00  1.769E+04   !2
corrected to ag
EP+R8CH3OO=EPEJ+CH3OOH                7.220E+03   2.55  1.053E+04
EP+R8CH3OO=EPMJ+CH3OOH                8.400e+12   0.00  2.044e+04   !2
corrected to ag

EP3J=EPEJ                           9.872e+07   1.00  2.000e+04   !(cyc
lact sat a 6 + 2Hs - 2kcal/O)
EP2J=EPMJ                           1.481e+08   1.00  2.450e+04   !(cyc
lact sat a 6 + 3Hp)
EP2J=EPEJ                           5.746e+08   1.00  1.800e+04   !(cyc
lact sat a 5 + 2Hs - 2kcal/O)
!EPMJ=EP2J    9.9E+0007  1.000  12000.0  ! IS 26 KB
!EPMJ=EP3J    1.7E+0007  1.000  17400.0  ! IS 27 KB
!EPEJ=EP2J    5.7E+0008  1.000  21300.0  ! IS 28 KB
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!EPEJ=EP3J    9.9E+0007  1.000  18000.0  ! IS 29 KB

!EP3J+O2=EP3oo                      9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!!EP2J+O2=EP2oo                      1.000e+19  -2.50  0.000e+00   !Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EP2J+O2=EP2oo                      1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPEJ+O2=EPEoo                      1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPMJ+O2=EPmoo                      9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!
!EP3oo=EP2d+R3OOH                   5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EP2oo=EP2d+R3OOH                   5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPEoo=EPED+R3OOH                   5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPmoo=EPED+R3OOH                   5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal

!EP3J=C2H4Z+C2H5OCO                  8.827E+15  -0.67  3.555E+04
EP3J=C2H4Z+C2H5OCO                  3.030E+13   0.27    34667.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!EP2J=CH3CHCO+R15C2H5O               2.786E+22  -2.31  4.566E+04
EP2J=CH3CHCO+R15C2H5O               1.460E+12   0.61    53276.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EPEJ=CH3CHO+R25C2H5CO                1.127E+21  -1.73  4.255E+04   !
+2kcal
EPEJ=CH3CHO+R25C2H5CO                1.127E+21  -1.73  4.255E+04   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EPMJ=C2H4Z+C2H5CO2                 2.325E+14  -0.20  3.297E+04
EPMJ=C2H4Z+C2H5CO2                  1.340E+13  -0.40  2.461E+04  !
Westbrook et al., (2009)
MPMJ=HCHO+R25C2H5CO                  1.230E+13   0.375   36714.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!EP3J*o=>EA2J+B2CO                   1.834e+15  -0.73  1.291e+04   !
Glaude et al., DMC C2H5CO
!EP3J2*o=CH2COZ  +C2H5OCO             1.230E+13   0.375   36714.0   !
Huynh and Violi J.Org.Chem. 73 (2008) 94-101

EP3J=EP2d+R1H                        3.000e+13   0.00  3.800e+04  !ST
EP2J=EP2d+R1H                        3.000e+13   0.00  3.900e+04  !ST
EPEJ=EPED+R1H                        3.000e+13   0.00  3.900e+04  !ST
EPMJ=EPED+R1H                        3.000e+13   0.00  3.800e+04  !ST

!EP3J+O2=EP2d+R3OOH                 2.600E+11   0.00  2.500E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EP2J+O2=EP2d+R3OOH                 1.580E+12   0.00  1.520E+04   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EP3J+O2=EP2d+R3OOH                 1.580E+12   0.00  5.000E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
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!EP2J+O2=EP2d+R3OOH                1.580E+12   0.00  5.000E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPEJ+O2=EPED+R3OOH                1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPMJ+O2=EPED+R3OOH                1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EP3J+R3OOH=EP2d+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EP2J+R3OOH=EP2d+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPEJ+R3OOH=EPED+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPMJ+R3OOH=EPED+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)

!C2H5COOH=CH2COOH+R4CH3              3.981E+15   0.00  8.852E+04   !
Doolan et al., Int.J.Chem.Kinet. 18 (1986) 575-596
!C2H5COOH=HOCO+R11C2H5               1.995E+15   0.00  8.612E+04   !Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596
!C2H5COOH=CH3CHCO+H2O               7.079E+12   0.00  7.057E+04   !Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596
!C2H5COOH=C2H6+CO2                  5.012E+12   0.00  7.177E+04   !Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596
C2H5COOH=CH3CHCO+H2O               4.470E+14   0.00  7.989E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C2H5COOH=C2H6+CO2                  7.080E+13   0.00  7.452E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C2H5COOH=>R25C2H5CO+R2OH              1.4E+0017   0.000  105815.7  ! UI
8 KB
C2H5COOH=>C2H5CO2+R1H               2.3E+0014   0.000  106345.3  ! UI 9
KB
C2H5COOH=>R11C2H5   +HOCO              8.2E+0016   0.000   88817.0  ! UI
10 KB
C2H5COOH=>R4CH3+CH2COOH             2.9E+0016   0.000   81917.1  ! UI 11
KB +3kcal

C2H5COOH+R1H=CH2CH2COOH+H2          9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
C2H5COOH+R1H=CH3CHCOOH+H2           1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
!C2H5COOH+R1H=CH3CHCOOH+H2           5.400e+04   2.5  -1.900e+03   !
!C2H5COOH+R1H=C2H5CO2+H2             4.2E+0006   2.000    2400.0   ! ME
96 CN
C2H5COOH+R1H=C2H5CO2+H2             5.550E-23   10.60   -4459.0   !
PARk,Zhu,Lin, JcP 118, 9990-9996 (2003)
C2H5COOH+B1O=CH2CH2COOH+R2OH          9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
C2H5COOH+B1O=CH3CHCOOH+R2OH           4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
!C2H5COOH+B1O=CH3CHCOOH+R2OH           8.800e+10   0.70  3.250e+03   !
!C2H5COOH+B1O=C2H5CO2+R2OH             1.0E+0013   0.000    3280.0   ! ME
87 CW
C2H5COOH+B1O=C2H5CO2+R2OH             1.460E-03    4.73    1727.0   ! Wu,
Lee, Xu, Lin, JPcA 2007
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C2H5COOH+R2OH=CH2CH2COOH+H2O        5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
C2H5COOH+R2OH=CH3CHCOOH+H2O         4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
!C2H5COOH+R2OH=CH3CHCOOH+H2O         3.000e+06   2.00 -1.520e+03   !
!C2H5COOH+R2OH=C2H5CO2+H2O           1.1E+0006   2.000   -1865.0   ! ME
105 CW
C2H5COOH+R2OH=C2H5CO2+H2O           2.810E+02    2.97    -580.0   ! Xu
Lin pci 2007 31 159-166
C2H5COOH+R4CH3=CH2CH2COOH+CH4       4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
C2H5COOH+R4CH3=CH3CHCOOH+CH4        2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
!C2H5COOH+R4CH3=CH3CHCOOH+CH4        1.000e+11   0.00  7.300e+03   !
C2H5COOH+R4CH3=C2H5CO2+CH4          2.035E+00    3.57    7722.0   !
Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
C2H5COOH+R3OOH=CH2CH2COOH+H2O2      8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C2H5COOH+R3OOH=>CH3CHCOOH+H2O2       5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!C2H5COOH+R3OOH=CH3CHCOOH+H2O2       6.400e+03   2.60  1.240e+04   !
!C2H5COOH+R3OOH=C2H5CO2+H2O2         2.11E+0006  0.000   14000.0   ! ME
96 CN
C2H5COOH+R3OOH=C2H5CO2+H2O2         2.500E+12    0.00   24000.0 ! MARinov
1998
C2H5COOH+R8CH3OO=CH2CH2COOH+CH3OOH  8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C2H5COOH+R8CH3OO=CH3CHCOOH+CH3OOH   5.600E+12   0.00  1.769E+04   !2
corrected to ag
!C2H5COOH+R8CH3OO=CH3CHCOOH+CH3OOH   6.400e+03   2.60  1.240e+04   !
C2H5COOH+R7CH3O  =CH2CH2COOH+CH3OH    1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
C2H5COOH+R7CH3O  =CH3CHCOOH+CH3OH     1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
!C2H5COOH+R7CH3O  =CH3CHCOOH+CH3OH     1.780e+12   0.00  1.200e+03   !

CH2CH2COOH=C2H4Z+HOCO              3.030E+13   0.27    34667.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!CH2CH2COOH=C2H4Z+HOCO              4.217E+14  -0.32  3.486E+04
CH2CH2COOH=C2H3COOH+R1H             3.200E+13   0.00    34800.0   !ST
CH3CHCOOH=CH3CHCO+R2OH              3.046E+21  -1.61  5.730E+04
CH3CHCOOH=C2H3COOH+R1H              3.000E+13   0.00  5.150E+04   !ST
CH3CHCOOH=>CO2+R11C2H5               1.700E+09   1.0     38640.0
C2H3COOH+R2OH=>HCHO+CH2COOH         1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C2H3COOH+R2OH=>R4CH3+R5CHO+HOCO         1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C2H3COOH=R10C2H3V+HOCO               3.752E+21  -1.89  1.129E+05
C2H3COOH=CH2CHCO+R2OH               5.206E+20  -1.16  1.009E+05
C2H3COOH=C2H4Z+CO2                 7.080E+13   0.00  7.452E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
!C2H3COOH=C2H4Z+CO2                 5.012E+12   0.00  7.177E+04   !Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596
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C2H3COOH+R1H=>H2+CO2+R10C2H3V           4.2E+0006  2.100  6900.0  ! MZB
483
C2H3COOH+R2OH=>H2O+CO2+R10C2H3V         5.4E+0004  2.000  -340.0  ! MZB
484
C2H3COOH+R3OOH=>H2O2+CO2+R10C2H3V       1.0E+0011  0.000  11500.0  ! MZB
485
C2H3COOH+R4CH3=>CH4+CO2+R10C2H3V        1.4E+0001  3.100  9940.0  ! MZB
486
C2H3COOH+R11C2H5   =>C2H6+CO2+R10C2H3V      1.4E+0001  3.100  8940.0  !
MZB 487
!C2H5CO2+m=R11C2H5   +CO2+m              4.400E+15   0.00  1.050E+04
CH3CHCO+R2OH=CH3CHO+R5CHO           1.000E+12   0.00        0.0   !Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596
EP2d+R2OH=>HCHO+EA2J                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPED+R2OH=>HCHO+MPMJ                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPED+R2OH=>CH3CHO+C2H5CO2           1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EP2d=C2H3COOH+C2H4Z                  2.000E+12   0.00  4.729E+04
!EP2d(+m)=C2H3COOH+C2H4Z(+m)        1.000E+13   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
!end
!EP3*o+R1H=EP3J*o+H2                1.200E+14   0.00     7000.0   !
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!EP3*o+B1O=EP3J*o+R2OH                5.850E+12   0.00     1808.0   !
(BAULch92)
!EP3*o+R2OH=EP3J*o+H2O               2.650E+12   0.00     -730.0   !
Atkinson et al., 2001
!EP3*o+R3OOH=EP3J*o+H2O2             1.700E+12    0.00   10700.0   !
(COLKET 77; CH3CHO)         3.100E+12   0.00    11920.0   !(BAULch92)
!EP3*o=choCH2COOH+C2H4Z            2.000E+12   0.00  4.729E+04
!choCH2COOH+R1H=coCH2COOH+H2                 1.200E+14   0.00     7000.0
!Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!choCH2COOH+B1O=coCH2COOH+R2OH                5.850E+12   0.00     1808.0
!(BAULch92)
!choCH2COOH+R2OH=coCH2COOH+H2O               2.650E+12   0.00     -730.0
!Atkinson et al., 2001
!choCH2COOH+R3OOH=coCH2COOH+H2O2             1.700E+12    0.00   10700.0
!(COLKET 77; CH3CHO)         3.100E+12   0.00    11920.0   !(BAULch92)
!coCH2COOH=>cH2co+B2CO+R2OH                   3.046E+21  -1.61  5.730E+04

EB=C3H7COOH+C2H4Z                   2.000E+12   0.00  4.729E+04
!EB(+m)=C3H7COOH+C2H4Z(+m)           4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
EB4J+R1H(+m)=EB(+m)                 1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EB3J+R1H(+m)=EB(+m)                 1.000E+14   0.00  0.000E+00
```

```
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EB2J+R1H(+m)=EB(+m)                1.000E+14   0.00  0.000E+00
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /
TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off
reaction
EBEJ+R1H(+m)=EB(+m)                1.000E+14   0.00  0.000E+00
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off
reaction
EBMJ+R1H(+m)=EB(+m)                1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EB(+m)=EP3J+R4CH3(+m)               7.213E+18  -0.89  8.721E+04   !asMB
LOW / 1.3080E+70 -1.5160E+01 8.4910E+04 /
TROE / 1.5409E-01 3.3770E+02 5.6730E+09 6.7100E+09 / !Troe Fall-off
reaction
EB(+m)=EA2J+R11C2H5   (+m)             2.700E+22  -1.86  8.568E+04   !
asMB
LOW / 3.9100E+74 -1.6420E+01 8.3700E+04 /
TROE / 8.6980E-01 7.4990E+09 1.6303E+00 7.5960E+07 / !Troe Fall-off
reaction
EB(+m)=C2H5OCO+R19C3H7(+m)         2.627E+27  -3.23  9.469E+04
LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /
TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off
reaction
EB(+m)=NC3H7CO+R15C2H5O(+m)       1.650E+24  -2.04  1.002E+05
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off
reaction
EB(+m)=C3H7CO2+R11C2H5   (+m)          5.734E+25  -2.76  9.211E+04
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off
reaction
EB(+m)=MBMJ+R4CH3(+m)              3.388E+21  -1.58  9.209E+04
LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /
TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off
reaction
EB+O2=EB4J+R3OOH                 3.000E+13   0.00  5.229E+04
EB+O2=EB3J+R3OOH                 4.000E+13   0.00  4.769E+04   !Tsang et
al., J. Phys. Chem. REF. Data 17 (1988) 887-
EB+O2=EB2J+R3OOH                 2.000E+13   0.00  4.430E+04
EB+O2=EBEJ+R3OOH                 2.000E+13   0.00  4.820E+04
EB+O2=EBMJ+R3OOH                 3.000E+13   0.00  5.229E+04

EB+R1H=EB4J+H2                     9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EB+R1H=EB3J+H2                     1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
EB+R1H=EB2J+H2                     1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
!EB+R1H=EB2J+H2                     5.400e+04   2.5  -1.900e+03   !
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EB+R1H=EBEJ+H2                      1.790E+05   2.53  3.420E+03   !as
C2H5OH PARk et al., J.Chem.Phys. 118 (2003) 9990-9996
EB+R1H=EBMJ+H2                      9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EB+B1O=EB4J+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EB+B1O=EB3J+R2OH                      4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
EB+B1O=EB2J+R2OH                      4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
!EB+B1O=EB2J+R2OH                      8.800e+10   0.70  3.250e+03   !
EB+B1O=EBEJ+R2OH                      1.450E+05   2.47  8.800E+02   !as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703
EB+B1O=EBMJ+R2OH                      9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EB+R2OH=EB4J+H2O                    5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EB+R2OH=EB3J+H2O                    4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
EB+R2OH=EB2J+H2O                    4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
!EB+R2OH=EB2J+H2O                     3.000e+06   2.00 -1.520e+03   !
EB+R2OH=EBEJ+H2O                    1.306E+05   2.43    -1457.0   !as
C2H5OH Xu Lin pci 2007 31 159-166
EB+R2OH=EBMJ+H2O                    5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EB+R4CH3=EB4J+CH4                   4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EB+R4CH3=EB3J+CH4                   2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
EB+R4CH3=EB2J+CH4                   2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
!EB+R4CH3=EB2J+CH4                    1.000e+11   0.00  7.300e+03   !
EB+R4CH3=EBEJ+CH4                   1.990E+01   3.37     7635.0   !as
C2H5OH Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
EB+R4CH3=EBMJ+CH4                   4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EB+R3OOH=EB4J+H2O2                  8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EB+R3OOH=EB3J+H2O2                  5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
EB+R3OOH=EB2J+H2O2                  5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!EB+R3OOH=EB2J+H2O2                   6.400e+03   2.60  1.240e+04   !
!EB+R3OOH=EBEJ+H2O2                   8.200E+03   2.55    10750.0   !
MARinov 1998
EB+R3OOH=EBEJ+H2O2                  3.610E+03   2.55  1.053E+04
EB+R3OOH=EBMJ+H2O2                  8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EB+R8CH3OO=EB4J+CH3OOH              8.400e+12   0.00  2.044e+04   !2
corrected to ag
EB+R8CH3OO=EB3J+CH3OOH              5.600E+12   0.00  1.769E+04   !2
corrected to ag
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EB+R8CH3OO=EB2J+CH3OOH              5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EB+R8CH3OO=EB2J+CH3OOH             6.400e+03   2.60  1.240e+04   !
EB+R8CH3OO=EBEJ+CH3OOH              7.220E+03   2.55  1.053E+04
EB+R8CH3OO=EBMJ+CH3OOH              8.400e+12   0.00  2.044e+04   !2
corrected to ag
EB+R7CH3O  =EB4J+CH3OH                1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
EB+R7CH3O  =EB3J+CH3OH                1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
EB+R7CH3O  =EB2J+CH3OH                1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
!EB+R7CH3O  =EB2J+CH3OH               1.780e+12   0.00  1.200e+03   !
EB+R7CH3O  =EBEJ+CH3OH                4.580E+10   0.00  2.873E+03
EB+R7CH3O  =EBMJ+CH3OH                1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;

EB3J=EBEJ                           9.872e+07   1.00  2.000e+04   !(cyc
lact sat a 6 + 2Hs - 2kcal/O)
EB2J=EBMJ                           1.481e+08   1.00  2.450e+04   !(cyc
lact sat a 6 + 3Hp)
EB2J=EBEJ                           5.746e+08   1.00  1.800e+04   !(cyc
lact sat a 5 + 2Hs - 2kcal/O)
!EB4J=EB2J    3.3E+0009  1.000  35000.0  ! IS 23 KB
!EB4J=EBEJ    1.7E+0007  1.000  15400.0  ! IS 24 KB
!EB4J=EBMJ    4.4E+0006  1.000  23400.0  ! IS 25 KB
!rev/ 4.4E+0006  1.000  23400.0/  ! IS 25 KB
!EBMJ=EB2J    9.9E+0007  1.000  12000.0  ! IS 26 KB
!EBMJ=EB3J    1.7E+0007  1.000  17400.0  ! IS 27 KB
!EBEJ=EB2J    5.7E+0008  1.000  21300.0  ! IS 28 KB
!EBEJ=EB3J    9.9E+0007  1.000  18000.0  ! IS 29 KB

!EB4J+O2=EB4oo                       9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!EB3J+O2=EB3oo                       1.700e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!!EB2J+O2=EB2oo                      1.000e+19  -2.50  0.000e+00   !Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EB2J+O2=EB2oo                       1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EBEJ+O2=EBeoo                       1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EBMJ+O2=EBmoo                       9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!
!EB4oo=EB3D+R3OOH                    5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EB3oo=EB3D+R3OOH                    5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EB3oo=EB2D+R3OOH                    5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EB2oo=EB2D+R3OOH                    5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
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!EBeoo=EBed+R3OOH                   5.075E+42  -9.410 4.249E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EBmoo=EBed+R3OOH                   5.044E+38  -8.110 4.149E+04 !Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal

EB4J=C2H4Z+EA2J                     5.250E+11   0.50    26591.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB4J=C2H4Z+EA2J                     2.100E+13   0.00    27800.0   !
EB3J=C3H6Y+C2H5OCO                  4.530E+12   0.335   34269.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB3J=C3H6Y+C2H5OCO                   8.827E+15  -0.67  3.555E+04
!EB3J=C3H6Y+C2H5OCO                   2.100E+13   0.00    31200.0   !
!EB2J=C2H5CHCO+R15C2H5O               2.786E+22  -2.31  4.566E+04
!EB2J=C2H5CHCO+R15C2H5O               2.100E+13   0.00    49000.0   !
EB2J=C2H5CHCO+R15C2H5O               1.460E+12   0.61    53276.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB2J=EP2d+R4CH3                      2.000E+13   0.00  3.700E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285 +6kcal
EB2J=EP2d+R4CH3                      1.330E+11    0.97   34882.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!EBEJ=CH3CHO+NC3H7CO                1.127E+21  -1.73  4.055E+04
!EBEJ=CH3CHO+NC3H7CO                2.100E+13   0.00    31900.0   !
EBEJ=CH3CHO+NC3H7CO                1.127E+21  -1.73  4.255E+04   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
EBMJ=C2H4Z+C3H7CO2                  2.325E+14  -0.20  3.297E+04
!EBMJ=C2H4Z+C3H7CO2                  2.100E+13   0.00  2.510E+04
MBMJ=HCHO+NC3H7CO                  1.230E+13   0.375   36714.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB4J*o=>EP3J+B2CO                    1.834e+15  -0.73  1.291e+04   !
Glaude et al., DMC C2H5co
!EB4J3*o=CH2COZ  +EA2J                1.230E+13   0.375   36714.0   !
Huynh and Violi J.Org.Chem. 73 (2008) 94-101
!EB4J2*o=>C2H4Z+EA2J*o               1.230E+13   0.375   36714.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101

EB4J=EB3D+R1H                        3.000e+13   0.00  3.800e+04  !ST
EB3J=EB3D+R1H                        3.000e+13   0.00  3.900e+04  !ST
EB3J=EB2D+R1H                        3.000e+13   0.00  3.800e+04  !ST
EB2J=EB2D+R1H                        3.000e+13   0.00  3.800e+04  !ST
EBEJ=EBed+R1H                        3.000e+13   0.00  3.900e+04  !ST
EBMJ=EBed+R1H                        3.000e+13   0.00  3.800e+04  !ST

!EB4J+O2=EB3D+R3OOH                 1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB3J+O2=EB3D+R3OOH                 1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB3J+O2=EB2D+R3OOH                 2.600E+11   0.00  2.500E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB2J+O2=EB2D+R3OOH                 1.580E+12   0.00  1.520E+04   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!!EB3J+O2=EB2D+R3OOH                 1.580E+12   0.00  5.000E+03   !
Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!!EB2J+O2=EB2D+R3OOH                 1.580E+12   0.00  5.000E+03   !
Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
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!EBEJ+O2=EBed+R3OOH                1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EBMJ+O2=EBed+R3OOH                1.580E+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB4J+R3OOH=EB3D+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EB3J+R3OOH=EB3D+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EB3J+R3OOH=EB2D+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EB2J+R3OOH=EB2D+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EBEJ+R3OOH=EBed+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EBMJ+R3OOH=EBed+H2O2                2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)

C3H7COOH=C2H5CHCO+H2O             4.470E+14   0.00  7.989E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C3H7COOH=C3H8+CO2                 7.080E+13   0.00  7.452E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C3H7COOH=>NC3H7CO+R2OH              1.4E+0017   0.000  105815.7  ! UI 8
KB
C3H7COOH=>C3H7CO2+R1H               2.3E+0014   0.000  106345.3  ! UI 9
KB
C3H7COOH=>R19C3H7+HOCO              8.2E+0016   0.000   88817.0  ! UI 10
KB
C3H7COOH=>R11C2H5   +CH2COOH           2.9E+0016   0.000   78917.1  ! UI
11 KB
C3H7COOH=>R4CH3+CH2CH2COOH          1.7E+0017   0.000   87662.1  ! UI 12
KB

C3H7COOH+R1H=PRCOOH-4+H2            9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
C3H7COOH+R1H=PRCOOH-3+H2            1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
C3H7COOH+R1H=PRCOOH-2+H2            1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
!C3H7COOH+R1H=PRCOOH-2+H2            5.400e+04   2.5  -1.900e+03   !
!C3H7COOH+R1H=C3H7CO2+H2             4.2E+0006   2.000    2400.0   ! ME
96 CN
C3H7COOH+R1H=C3H7CO2+H2             5.550E-23   10.60   -4459.0   !
PARk,Zhu,Lin, JcP 118, 9990-9996 (2003)
C3H7COOH+B1O=PRCOOH-4+R2OH            9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
C3H7COOH+B1O=PRCOOH-3+R2OH            4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
C3H7COOH+B1O=PRCOOH-2+R2OH            4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
!C3H7COOH+B1O=PRCOOH-2+R2OH            8.800e+10   0.70  3.250e+03   !
!C3H7COOH+B1O=C3H7CO2+R2OH             1.0E+0013   0.000    3280.0   ! ME
87 CW
C3H7COOH+B1O=C3H7CO2+R2OH             1.460E-03    4.73    1727.0   ! Wu,
Lee, Xu, Lin, JPcA 2007
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C3H7COOH+R2OH=PRCOOH-4+H2O          5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
C3H7COOH+R2OH=PRCOOH-3+H2O          4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
C3H7COOH+R2OH=PRCOOH-2+H2O          4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
!C3H7COOH+R2OH=PRCOOH-2+H2O          3.000e+06   2.00 -1.520e+03   !
!C3H7COOH+R2OH=C3H7CO2+H2O           1.1E+0006   2.000   -1865.0   ! ME
105 CW
C3H7COOH+R2OH=C3H7CO2+H2O           2.810E+02    2.97    -580.0   ! Xu
Lin pci 2007 31 159-166
C3H7COOH+R4CH3=PRCOOH-4+CH4         4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
C3H7COOH+R4CH3=PRCOOH-3+CH4         2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
C3H7COOH+R4CH3=PRCOOH-2+CH4         2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
!C3H7COOH+R4CH3=PRCOOH-2+CH4         1.000e+11   0.00  7.300e+03   !
C3H7COOH+R4CH3=C3H7CO2+CH4          2.035E+00    3.57    7722.0   !
Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
C3H7COOH+R3OOH=PRCOOH-4+H2O2        8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C3H7COOH+R3OOH=PRCOOH-3+H2O2        5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
C3H7COOH+R3OOH=>PRCOOH-2+H2O2        5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!C3H7COOH+R3OOH=PRCOOH-2+H2O2        6.400e+03   2.60  1.240e+04   !
!C3H7COOH+R3OOH=C3H7CO2+H2O2         2.11E+0006  0.000   14000.0   ! ME
96 CN
C3H7COOH+R3OOH=C3H7CO2+H2O2         2.500E+12    0.00   24000.0 ! MARinov
1998
C3H7COOH+R8CH3OO=PRCOOH-4+CH3OOH    8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C3H7COOH+R8CH3OO=PRCOOH-3+CH3OOH    5.600E+12   0.00  1.769E+04   !2
corrected to ag
C3H7COOH+R8CH3OO=PRCOOH-2+CH3OOH    5.600E+12   0.00  1.769E+04   !2
corrected to ag
!C3H7COOH+R8CH3OO=PRCOOH-2+CH3OOH    6.400e+03   2.60  1.240e+04   !
C3H7COOH+R7CH3O  =PRCOOH-4+CH3OH      1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
C3H7COOH+R7CH3O  =PRCOOH-3+CH3OH      1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
C3H7COOH+R7CH3O  =PRCOOH-2+CH3OH      1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
!C3H7COOH+R7CH3O  =PRCOOH-2+CH3OH      1.780e+12   0.00  1.200e+03   !

PRCOOH-4=C2H4Z+CH2COOH             5.250E+11   0.50    26591.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
PRCOOH-3=C3H6Y+HOCO                3.030E+13   0.27    34667.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!PRCOOH-3=C3H6Y+HOCO                4.217E+14  -0.32  3.486E+04
PRCOOH-2=C2H3COOH+R4CH3             1.330E+11   0.97    34882.0   !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
PRCOOH-2=C2H5CHCO+R2OH              3.046E+21  -1.61  5.730E+04
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PRCOOH-2=>CO2+R19C3H7          1.700E+09   1.0     38640.0
!PRCOOH-4=C2H4Z+CH2COOH            2.000E+13   0.00    28700.0   !
!PRCOOH-3=C3H6Y+HOCO               2.000E+13   0.00    28700.0   !
!PRCOOH-2=C2H3COOH+R4CH3            2.000E+13   0.00    31000.0   !
!PRCOOH-2=C2H5CHCO+R2OH             2.000E+13   0.00    49000.0   !
C3H7CO2+m=R19C3H7+CO2+m            4.400E+15   0.00  1.050E+04
!C3H7CO2=R19C3H7+CO2             2.000E+13   0.00  5.100E+03
PRCOOH-4=C3H5COOH+R1H              3.000E+13   0.00    38000.0   !ST
PRCOOH-3=C3H5COOH+R1H              3.200E+13   0.00    34800.0   !ST
PRCOOH-2=C3H5COOH+R1H              3.000E+13   0.00  5.150E+04   !ST
C3H5COOH+R2OH=>HCHO+CH2CH2COOH     1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C3H5COOH+R2OH=>CH3CHO+CH2COOH      1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C3H5COOH+R1H=>H2+CO2+sC3H5         4.2E+0006  2.100  6900.0  ! MZB 483
C3H5COOH+R2OH=>H2O+CO2+sC3H5       5.4E+0004  2.000  -340.0  ! MZB 484
C3H5COOH+R3OOH=>H2O2+CO2+sC3H5     1.0E+0011  0.000  11500.0  ! MZB 485
C3H5COOH+R4CH3=>CH4+CO2+sC3H5      1.4E+0001  3.100  9940.0  ! MZB 486
C3H5COOH+R11C2H5   =>C2H6+CO2+sC3H5    1.4E+0001  3.100  8940.0  ! MZB
487
EB3D+R2OH=>HCHO+EP3J               1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EB3D+R2OH=>CH3CHO+EA2J             1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EB2D+R2OH=>CH3CHO+EA2J             1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EBed+R2OH=>HCHO+MBMJ               1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EBed+R2OH=>CH3CHO+C3H7CO2          1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EB3D=C3H5COOH+C2H4Z               2.000E+12   0.00  4.729E+04
EB2D=C3H5COOH+C2H4Z               2.000E+12   0.00  4.729E+04
!EB3D(+m)=C3H5COOH+C2H4Z(+m)        4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction

!EB4*o+R1H=EB4J*o+H2               1.200E+14   0.00     7000.0   !
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!EB4*o+B1O=EB4J*o+R2OH              5.850E+12   0.00     1808.0   !
(BAULch92)
!EB4*o+R2OH=EB4J*o+H2O              2.650E+12   0.00     -730.0   !
Atkinson et al., 2001
!EB4*o+R3OOH=EB4J*o+H2O2            1.700E+12    0.00   10700.0   !
(COLKET 77; CH3CHO)         3.100E+12   0.00    11920.0   !(BAULch92)

EPE=C4H9COOH+C2H4Z                2.000E+12   0.00  4.729E+04
!EPE(+m)=C4H9COOH+C2H4Z(+m)         4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
EPE5J+R1H(+m)=EPE(+m)              1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
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TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EPE4J+R1H(+m)=EPE(+m)               1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EPE3J+R1H(+m)=EPE(+m)               1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EPE2J+R1H(+m)=EPE(+m)               1.000E+14   0.00  0.000E+00
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /
TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off
reaction
EPEEJ+R1H(+m)=EPE(+m)               1.000E+14   0.00  0.000E+00
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off
reaction
EPEMJ+R1H(+m)=EPE(+m)               1.000E+14   0.00  0.000E+00
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off
reaction
EPE(+m)=EB4J+R4CH3(+m)              7.213E+18  -0.89  8.721E+04   !asMB
LOW / 1.3080E+70 -1.5160E+01 8.4910E+04 /
TROE / 1.5409E-01 3.3770E+02 5.6730E+09 6.7100E+09 / !Troe Fall-off
reaction
EPE(+m)=EP3J+R11C2H5   (+m)             5.732E+23  -2.33  8.774E+04
LOW / 4.3520E+14 8.2000E-01 6.3570E+04 /
TROE / 1.6900E-01 5.7129E+03 4.0466E+01 6.7101E+09 / !Troe Fall-off
reaction
EPE(+m)=EA2J+R19C3H7(+m)            2.700E+22  -1.86  8.568E+04   !asMB
LOW / 3.9100E+74 -1.6420E+01 8.3700E+04 /
TROE / 8.6980E-01 7.4990E+09 1.6303E+00 7.5960E+07 / !Troe Fall-off
reaction
EPE(+m)=C2H5OCO+R20C4H9(+m)         2.627E+27  -3.23  9.469E+04
LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /
TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off
reaction
EPE(+m)=NC4H9CO+R15C2H5O(+m)       1.650E+24  -2.04  1.002E+05
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off
reaction
EPE(+m)=C4H9CO2+R11C2H5   (+m)          5.734E+25  -2.76  9.211E+04
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off
reaction
EPE(+m)=MPEMJ+R4CH3(+m)             3.388E+21  -1.58  9.209E+04
LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /
TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off
reaction
EPE+O2=EPE5J+R3OOH                3.000E+13   0.00  5.229E+04
EPE+O2=EPE4J+R3OOH                4.000E+13   0.00  4.769E+04   !Tsang et
al., J. Phys. Chem. REF. Data 17 (1988) 887-
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EPE+O2=EPE3J+R3OOH                4.000E+13   0.00  4.769E+04   !Tsang et
al., J. Phys. Chem. REF. Data 17 (1988) 887-
EPE+O2=EPE2J+R3OOH                2.000E+13   0.00  4.430E+04
EPE+O2=EPEEJ+R3OOH                2.000E+13   0.00  4.820E+04
EPE+O2=EPEMJ+R3OOH                3.000E+13   0.00  5.229E+04

EPE+R1H=EPE5J+H2                    9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EPE+R1H=EPE4J+H2                    1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
EPE+R1H=EPE3J+H2                    1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
EPE+R1H=EPE2J+H2                    1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
!EPE+R1H=EPE2J+H2                    5.400e+04   2.5  -1.900e+03
EPE+R1H=EPEEJ+H2                    1.794E+05   2.53  3.420E+03   !as
C2H5OH PARk et al., J.Chem.Phys. 118 (2003) 9990-9996
EPE+R1H=EPEMJ+H2                    9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
EPE+B1O=EPE5J+R2OH                    9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EPE+B1O=EPE4J+R2OH                    4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
EPE+B1O=EPE3J+R2OH                    4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
EPE+B1O=EPE2J+R2OH                    4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
!EPE+B1O=EPE2J+R2OH                    8.800e+10   0.70  3.250e+03
EPE+B1O=EPEEJ+R2OH                    1.450E+05   2.41  8.760E+02   !as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703
EPE+B1O=EPEMJ+R2OH                    9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
EPE+R2OH=EPE5J+H2O                  5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EPE+R2OH=EPE4J+H2O                  4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
EPE+R2OH=EPE3J+H2O                  4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
EPE+R2OH=EPE2J+H2O                  4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
!EPE+R2OH=EPE2J+H2O                   3.000e+06   2.00 -1.520e+03
EPE+R2OH=EPEEJ+H2O                  1.306E+05   2.43    -1457.0   !as
C2H5OH Xu et al., Proc.Combust.Inst., 31 (2007) 159-166
EPE+R2OH=EPEMJ+H2O                  5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
EPE+R4CH3=EPE5J+CH4                 4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EPE+R4CH3=EPE4J+CH4                 2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
EPE+R4CH3=EPE3J+CH4                 2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
EPE+R4CH3=EPE2J+CH4                 2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
!EPE+R4CH3=EPE2J+CH4                  1.000e+11   0.00  7.300e+03
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EPE+R4CH3=EPEEJ+CH4                 1.990E+01   3.37     7635.0   !as
C2H5OH Xu et al., J.Chem.Phys., 120 (2004) 6593-6599
EPE+R4CH3=EPEMJ+CH4                 4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
EPE+R3OOH=EPE5J+H2O2                8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EPE+R3OOH=EPE4J+H2O2                5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
EPE+R3OOH=EPE3J+H2O2                5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
EPE+R3OOH=EPE2J+H2O2                5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!EPE+R3OOH=EPE2J+H2O2                6.400e+03   2.60  1.240e+04
!EPE+R3OOH=EPEEJ+H2O2                8.200E+03   2.55    10750.0   !
MARinov 1998
EPE+R3OOH=EPEEJ+H2O2                3.610E+03   2.55  1.053E+04
EPE+R3OOH=EPEMJ+H2O2                8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
EPE+R8CH3OO=EPE5J+CH3OOH            8.400e+12   0.00  2.044e+04   !2
corrected to ag
EPE+R8CH3OO=EPE4J+CH3OOH            5.600E+12   0.00  1.769E+04   !2
corrected to ag
EPE+R8CH3OO=EPE3J+CH3OOH            5.600E+12   0.00  1.769E+04   !2
corrected to ag
EPE+R8CH3OO=EPE2J+CH3OOH            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+R8CH3OO=EPE2J+CH3OOH            6.400e+03   2.60  1.240e+04
EPE+R8CH3OO=EPEEJ+CH3OOH            5.600e+12   0.00  1.769e+04   !2
corrected to ag
!EPE+R8CH3OO=EPEEJ+CH3OOH            7.220E+03   2.55  1.053E+04
EPE+R8CH3OO=EPEMJ+CH3OOH            8.400e+12   0.00  2.044e+04   !2
corrected to ag
EPE+R7CH3O  =EPE5J+CH3OH              1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
EPE+R7CH3O  =EPE4J+CH3OH              1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
EPE+R7CH3O  =EPE3J+CH3OH              1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
EPE+R7CH3O  =EPE2J+CH3OH              1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
!EPE+R7CH3O  =EPE2J+CH3OH               1.780e+12   0.00  1.200e+03
EPE+R7CH3O  =EPEEJ+CH3OH              4.580E+10   0.00  2.873E+03
EPE+R7CH3O  =EPEMJ+CH3OH              1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
!EPE+EPE5oo=EPE5J+EPE5ooh            8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE5oo=EPE4J+EPE5ooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE5oo=EPE3J+EPE5ooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE5oo=EPE2J+EPE5ooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE5oo=EPEEJ+EPE5ooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
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!EPE+EPE5oo=EPEMJ+EPE5ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE4oo=EPE5J+EPE4ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE4oo=EPE4J+EPE4ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE4oo=EPE3J+EPE4ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE4oo=EPE2J+EPE4ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE4oo=EPEEJ+EPE4ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE4oo=EPEMJ+EPE4ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE3oo=EPE5J+EPE3ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE3oo=EPE4J+EPE3ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE3oo=EPE3J+EPE3ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE3oo=EPE2J+EPE3ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE3oo=EPEEJ+EPE3ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE3oo=EPEMJ+EPE3ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE2oo=EPE5J+EPE2ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPE2oo=EPE4J+EPE2ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE2oo=EPE3J+EPE2ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE2oo=EPE2J+EPE2ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE2oo=EPEEJ+EPE2ooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPE2oo=EPEMJ+EPE2ooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPEeoo=EPE5J+EPEeooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPEeoo=EPE4J+EPEeooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEeoo=EPE3J+EPEeooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEeoo=EPE2J+EPEeooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEeoo=EPEEJ+EPEeooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEeoo=EPEMJ+EPEeooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPEmoo=EPE5J+EPEmooh           8.400e+12   0.00  2.044e+04   !2
corrected to ag
!EPE+EPEmoo=EPE4J+EPEmooh           5.600E+12   0.00  1.769E+04   !2
corrected to ag
```

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!EPE+EPEmoo=EPE3J+EPEmooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEmoo=EPE2J+EPEmooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEmoo=EPEEJ+EPEmooh            5.600E+12   0.00  1.769E+04   !2
corrected to ag
!EPE+EPEmoo=EPEMJ+EPEmooh            8.400e+12   0.00  2.044e+04   !2
corrected to ag

EPE2J=EPE5J                        8.619e+08   1.00  1.980e+04   !(cyc sat
a 5 + 3Hp)
EPE3J=EPEEJ                        9.872e+07   1.00  2.000e+04   !(cyc
lact sat a 6 + 2Hs - 2kcal/O)
EPE2J=EPEMJ                        1.481e+08   1.00  2.450e+04   !(cyc
lact sat a 6 + 3Hp)
EPE2J=EPEEJ                        5.746e+08   1.00  1.800e+04   !(cyc
lact sat a 5 + 2Hs - 2kcal/O)
!EPE4J=EPE2J    3.3E+0009  1.000  35000.0  ! IS 23 KB
!EPE4J=EPEEJ    1.7E+0007  1.000  15400.0  ! IS 24 KB
!EPE4J=EPEMJ    4.4E+0006  1.000  23400.0  ! IS 25 KB
!EPEMJ=EPE2J    9.9E+0007  1.000  12000.0  ! IS 26 KB
!EPEMJ=EPE3J    1.7E+0007  1.000  17400.0  ! IS 27 KB
!EPEEJ=EPE2J    5.7E+0008  1.000  21300.0  ! IS 28 KB
!EPEEJ=EPE3J    9.9E+0007  1.000  18000.0  ! IS 29 KB

!EPE5J+O2=EPE4D+R3OOH              1.580e+12   0.00  4.700e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE4J+O2=EPE4D+R3OOH              6.900e+11   0.00  4.700e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE4J+O2=EPE3D+R3OOH              1.580e+12   0.00  4.700e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE3J+O2=EPE3D+R3OOH              1.580e+12   0.00  4.700e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE3J+O2=EPE2D+R3OOH              2.600E+11   0.00  2.500E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE2J+O2=EPE2D+R3OOH              1.580E+12   0.00  1.520E+04   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE3J+O2=EPE2D+R3OOH              1.580E+12   0.00  5.000E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE2J+O2=EPE2D+R3OOH              1.580E+12   0.00  5.000E+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPEEJ+O2=EPEED+R3OOH              6.900e+11   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPEMJ+O2=EPEED+R3OOH              1.580e+12   0.00  5.000e+03   !Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EPE5J+R3OOH=EPE4D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPE4J+R3OOH=EPE4D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPE4J+R3OOH=EPE3D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPE3J+R3OOH=EPE3D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
```

```
!EPE3J+R3OOH=EPE2D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPE2J+R3OOH=EPE2D+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPEEJ+R3OOH=EPEED+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)
!EPEMJ+R3OOH=EPEED+H2O2              2.410E+13   0.0         0.0   !
(=R19C3H7/TSA88)

!EPE5J+O2=EPE5oo                    9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!EPE4J+O2=EPE4oo                    1.700e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!EPE3J+O2=EPE3oo                    1.800e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)
!!EPE2J+O2=EPE2oo                    1.000e+19  -2.50  0.000e+00   !Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPE2J+O2=EPE2oo                    1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!!EPEEJ+O2=EPEeoo                    1.700e+19  -2.50  0.000e+00   !Buda
et al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!EPEEJ+O2=EPEeoo                    1.200e+10   0.00    -2300.0   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPEMJ+O2=EPEmoo                    9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!
!EPE5oo=EPE5ooh4j                   5.746e+08   1.00  3.250e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)
!EPE5oo=EPE5ooh3j                   9.872e+07   1.00  2.500e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)
!EPE5oo=EPE5ooH2j                   1.696e+07   1.00  2.200e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 2Hs)
!EPE4oo=EPE4ooh5j                   8.619e+08   1.00  3.550e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 3Hp)
!EPE4oo=EPE4ooh3j                   5.746e+08   1.00  3.250e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)
!EPE4oo=EPE4ooH2j                   9.872e+07   1.00  2.500e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)
!EPE3oo=EPE3ooh5j                   1.481e+08   1.00  2.800e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 3Hp)
!EPE3oo=EPE3ooh4j                   5.746e+08   1.00  3.250e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)
!EPE3oo=EPE3ooH2j                   5.746e+08   1.00  3.250e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)
!EPE2oo=EPE2ooh5j                   2.544e+07   1.00  2.500e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 3Hp)
!EPE2oo=EPE2ooh4j                   9.872e+07   1.00  2.500e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)
!EPE2oo=EPE2ooh3j                   5.746e+08   1.00  3.250e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)
!EPE2oo=EPE2oohej                   1.696e+07   1.00  2.270e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs - 2kcal/O)
!EPEeoo=EPEeooH2j                   1.696e+07   1.00  2.550e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs)
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!EPEeoo=EPEeoohmj                  8.619e+08   1.00  3.550e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 3Hp)
!EPEmoo=EPEmoohej                  5.746e+08   1.00  3.050e+04   !Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)
!
!EPE5ooh4j+O2=EPE5ooh4oo           1.800e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)
!EPE5ooh3j+O2=EPE5ooh3oo           1.800e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)
!EPE5ooH2j+O2=EPE5ooH2Oo           1.000e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPE4ooh5j+O2=EPE4ooh5oo           1.500e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kt)
!EPE4ooh3j+O2=EPE4ooh3oo           1.050e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kt)
!EPE4ooH2j+O2=EPE4ooH2Oo           1.000e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPE3ooh5j+O2=EPE3ooh5oo           9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!EPE3ooh4j+O2=EPE3ooh4oo           9.500e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+kt)
!EPE3ooH2j+O2=EPE3ooH2Oo           2.500e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kt+kq)
!EPE2ooh5j+O2=EPE2ooh5oo           9.000e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)
!EPE2ooh4j+O2=EPE2ooh4oo           1.700e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!EPE2ooh3j+O2=EPE2ooh3oo           1.050e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kt)
!EPE2oohej+O2=EPE2ooheoo           1.700e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)
!EPEeooH2j+O2=EPEeooH2Oo           1.050e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)
!EPEeoohmj+O2=EPEeoohmoo           1.500e+18  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (kt)
!EPEmoohej+O2=EPEmooheoo           1.800e+19  -2.50  0.000e+00   !Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)
!
!EPE5ooh4oo=>EPE4ooh5*o+R2OH         5.746e+08   1.00  3.050e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)
!EPE5ooh3oo=>EPE3ooh5*o+R2OH         9.872e+07   1.00  2.300e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs - 2kcal/O)
!EPE5ooH2Oo=>EPE2ooh5*o+R2OH         1.696e+07   1.00  2.000e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 2Hs - 2kcal/O)
!EPE4ooh5oo=>EPE5ooh4*o+R2OH         2.873e+08   1.00  2.750e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)
!EPE4ooh3oo=>EPE3ooh4*o+R2OH         2.873e+08   1.00  2.750e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)
!EPE4ooH2Oo=>EPE2ooh4*o+R2OH         4.936e+07   1.00  2.000e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)
!EPE3ooh5oo=>EPE5ooh3*o+R2OH         4.936e+07   1.00  2.000e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)
!EPE3ooh4oo=>EPE4ooh3*o+R2OH         2.873e+08   1.00  2.750e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)
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!EPE3ooH2Oo=>EPE2ooh3*o+R2OH          2.873e+08   1.00  2.750e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)
!EPE2ooh5oo=>EPE5ooH2*o+R2OH          8.480e+06   1.00  1.700e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 1Ht - 2kcal/O)
!EPE2ooh4oo=>EPE4ooH2*o+R2OH          4.936e+07   1.00  2.000e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)
!EPE2ooh3oo=>EPE3ooH2*o+R2OH          2.873e+08   1.00  2.750e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)
!EPE2ooheoo=>EPEeooH2*o+R2OH          8.480e+06   1.00  2.350e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht -
2kcal/O)
!EPEeooH2Oo=>EPE2oohe*o+R2OH          8.480e+06   1.00  1.770e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht -
4kcal/O)
!EPEeoohmoo=>EPEmoohe*o+R2OH          2.873e+08   1.00  2.550e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 4kcal/O)
!EPEmooheoo=>EPEeoohm*o+R2OH          5.746e+08   1.00  3.050e+04   !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)
!
!EPE4ooh5*o=>CHOCHO+EP3J+R2OH        1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE3ooh5*o=>R13CH2CHO+EP3*o+R2OH       5.000e+15   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE3ooh5*o=>chocH2cho+EA2J+R2OH     5.000e+15   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE2ooh5*o=>choC2h4cho+C2H5OCO+R2OH 1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE5ooh4*o=>HCHO+EB4J*o+R2OH        1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE3ooh4*o=>R14CH3CO+EP3*o+R2OH        1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE2ooh4*o=>c4ald3oxo+C2H5OCO+R2OH  1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE5ooh3*o=>HCHO+EB4J3*o+R2OH       1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE4ooh3*o=>CH3CHO+EP3J*o+R2OH      1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE2ooh3*o=>c4ald2oxo+C2H5OCO+R2OH  5.000e+15   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE2ooh3*o=>ea2*o+R25C2H5CO+R2OH       5.000e+15   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE5ooH2*o=>HCHO+EB4J2*o+R2OH       1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE4ooH2*o=>CH3CHO+EP3J2*o+R2OH     1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE3ooH2*o=>C2H5CHO+EA2J*o+R2OH     1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPEeooH2*o=>CH3CHO+C3H7COCO2+R2OH   1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPE2oohe*o=>NC3H7CHO+CH3COCO2+R2OH  1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!EPEmoohe*o=>HCHO+MPEMJ*o+R2OH       1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
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!EPEeoohm*o=>C4H9CO2+CHOCHO+R2OH     1.000e+16   0.00  4.300e+04   !
Curran et al., Combust Flame, 114 (1998) 149-177
!
!EPE5ooh4j=>EPEcy5o4+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!EPE5ooh3j=>EPEcy5o3+R2OH             2.042e+11   0.00  1.950e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)
!EPE5ooH2j=>EPEcy5O2+R2OH             3.630e+10   0.00  1.300e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)
!EPE4ooh5j=>EPEcy5o4+R2OH             3.981e+12   0.00  1.700e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cp)
!EPE4ooh3j=>EPEcy4o3+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!EPE4ooH2j=>EPEcy4O2+R2OH             2.042e+11   0.00  1.950e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)
!EPE3ooh5j=>EPEcy5o3+R2OH             4.467e+11   0.00  2.190e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cp)
!EPE3ooh4j=>EPEcy4o3+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!EPE3ooH2j=>EPEcy3O2+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!EPE2ooh5j=>EPEcy5O2+R2OH             5.130e+10   0.00  1.480e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cp)
!EPE2ooh4j=>EPEcy4O2+R2OH             2.042e+11   0.00  1.950e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)
!EPE2ooh3j=>EPEcy3O2+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!EPE2oohej=>EPEcy2oe+R2OH             3.630e+10   0.00  1.300e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)
!EPEeooH2j=>EPEcy2oe+R2OH             3.630e+10   0.00  1.300e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)
!EPEeoohmj=>EPEcyeom+R2OH             3.981e+12   0.00  1.700e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cp)
!EPEmoohej=>EPEcyeom+R2OH             1.380e+12   0.00  1.590e+04   !
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)
!
!EPEcy5o4+R1H=>H2+C2H3CHOZ+EA2J        9.600E+08   1.50     2785.0   !25
dbr, see shee
!EPEcy5o4+R1H=>H2+CH2COZ  +EP3J          4.800E+08   1.50     2005.0   !
25  dbr, see shee
!EPEcy5o3+R1H=>H2+R5CHO+EB3D            9.600E+08   1.50     2785.0   !25
dbr, see shee
!EPEcy5o3+R1H=>H2+C2H4Z+EP3J*o         4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy5O2+R1H=>H2+R13CH2CHO+EP2d       9.600E+08   1.50     2785.0   !25
dbr, see shee
!EPEcy5O2+R1H=>H2+C2H4Z+EP3J2*o        4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy4o3+R1H=>H2+C2H3COCH3+C2H5OCO   4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy4o3+R1H=>H2+CH3CHCO+EA2J        4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy4O2+R1H=>H2+R14CH3CO+EP2d        4.800E+08   1.50     2005.0   !25
dbr, see shee
```

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!EPEcy4O2+R1H=>H2+C3H6Y+EA2J*o         4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy3O2+R1H=>H2+C2H5OCO+C2H5CHCO    9.600E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy2oe+R1H=>H2+B2CO+R14CH3CO+NC3H7CHO   4.800E+08   1.50
2005.0   !25  dbr, see shee
!EPEcy2oe+R1H=>H2+CH3CO2+C4H8CO       4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcy2oe+R1H=>H2+CH3CHO+prcoco       4.800E+08   1.50     2005.0   !25
dbr, see shee
!EPEcyeom+R1H=>H2+CHOCHO+NC4H9CO      9.600E+08   1.50     2785.0   !25
dbr, see shee
!EPEcyeom+R1H=>H2+CH2COZ  +C4H9CO2       4.800E+08   1.50     2005.0   !
25  dbr, see shee
!EPEcy5o4+R2OH=>H2O+C2H3CHOZ+EA2J      4.800E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy5o4+R2OH=>H2O+CH2COZ  +EP3J        2.400E+06   2.00    -1192.0   !
25  dbr, see shee
!EPEcy5o3+R2OH=>H2O+R5CHO+EB3D          4.800E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy5o3+R2OH=>H2O+C2H4Z+EP3J*o       2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy5O2+R2OH=>H2O+R13CH2CHO+EP2d     4.800E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy5O2+R2OH=>H2O+C2H4Z+EP3J2*o      2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy4o3+R2OH=>H2O+C2H3COCH3+C2H5OCO 2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy4o3+R2OH=>H2O+CH3CHCO+EA2J      2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy4O2+R2OH=>H2O+R14CH3CO+EP2d      2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy4O2+R2OH=>H2O+C3H6Y+EA2J*o       2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy3O2+R2OH=>H2O+C2H5OCO+C2H5CHCO  4.800E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy2oe+R2OH=>H2O+B2CO+R14CH3CO+NC3H7CHO 2.400E+06   2.00
-1192.0   !25  dbr, see shee
!EPEcy2oe+R2OH=>H2O+CH3CO2+C4H8CO     2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcy2oe+R2OH=>H2O+CH3CHO+prcoco     2.400E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcyeom+R2OH=>H2O+CHOCHO+NC4H9CO    4.800E+06   2.00    -1192.0   !25
dbr, see shee
!EPEcyeom+R2OH=>H2O+CH2COZ  +C4H9CO2     2.400E+06   2.00    -1192.0   !
25  dbr, see shee
!EPEcy5o4+R3OOH=>H2O2+C2H3CHOZ+EA2J    8.000E+12   0.00    14400.0   !25
my evans-po
!EPEcy5o4+R3OOH=>H2O2+CH2COZ  +EP3J      4.000E+12   0.00    13260.0   !
25  my evans-po
!EPEcy5o3+R3OOH=>H2O2+R5CHO+EB3D        8.000E+12   0.00    14400.0   !25
my evans-po
!EPEcy5o3+R3OOH=>H2O2+C2H4Z+EP3J*o     4.000E+12   0.00    13260.0   !25
my evans-po
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!EPEcy5O2+R3OOH=>H2O2+R13CH2CHO+EP2d   8.000E+12   0.00    14400.0   !25
my evans-po
!EPEcy5O2+R3OOH=>H2O2+C2H4Z+EP3J2*o    4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy4o3+R3OOH=>H2O2+C2H3COCH3+C2H5OCO 4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy4o3+R3OOH=>H2O2+CH3CHCO+EA2J    4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy4O2+R3OOH=>H2O2+R14CH3CO+EP2d    4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy4O2+R3OOH=>H2O2+C3H6Y+EA2J*o     4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy3O2+R3OOH=>H2O2+C2H5OCO+C2H5CHCO 8.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy2oe+R3OOH=>H2O2+B2CO+R14CH3CO+NC3H7CHO 4.000E+12   0.00    13260.0
!25  my evans-po
!EPEcy2oe+R3OOH=>H2O2+CH3CO2+C4H8CO   4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcy2oe+R3OOH=>H2O2+CH3CHO+prcoco   4.000E+12   0.00    13260.0   !25
my evans-po
!EPEcyeom+R3OOH=>H2O2+CHOCHO+NC4H9CO  8.000E+12   0.00    14400.0   !25
my evans-po
!EPEcyeom+R3OOH=>H2O2+CH2COZ  +C4H9CO2   4.000E+12   0.00    13260.0   !
25  my evans-po
!
!EPE5oo+R3OOH=EPE5ooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPE4oo+R3OOH=EPE4ooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPE3oo+R3OOH=EPE3ooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPE2oo+R3OOH=EPE2ooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPEeoo+R3OOH=EPEeooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPEmoo+R3OOH=EPEmooh+O2              2.110e+10   0.00    -3640.0   !
Anglada et al.,
!EPE5ooh=EPE5o+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPE4ooh=EPE4o+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPE3ooh=EPE3o+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPE2ooh=EPE2o+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPEeooh=EPEeo+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPEmooh=EPEmo+R2OH                   4.000e+15   0.00    42920.0   !
Baulch et al., (1994)
!EPE5o=HCHO+EB4J                    5.890e+13   0.00    13890.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE4o=R4CH3+EB4*o                    1.780e+13   0.00    14890.0   !
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275
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!EPE4o=CH3CHO+EP3J                  5.250e+13   0.00    11690.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE3o=R11C2H5   +EP3*o                  5.250e+13   0.00    11690.0   !
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE3o=C2H5CHO+EA2J                 5.250e+13   0.00    11690.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE2o=>R19C3H7+ea2*o                5.250e+13   0.00    11690.0   !
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE2o=NC3H7CHO+C2H5OCO             5.250e+13   0.00    11690.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPEeo=C4H9CO2+CH3CHO               5.250e+13   0.00    11690.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPEeo=mpem*o+R4CH3                  1.780e+13   0.00    14890.0   !
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPEmo=MPEMJ+HCHO                   5.890e+13   0.00    13890.0   !Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275
!EPE4D+R3OOH=EPE5ooh4j               2.470e+04   2.13  1.216e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPE4D+R3OOH=EPE4ooh5j               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPE3D+R3OOH=EPE4ooh3j               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPE3D+R3OOH=EPE3ooh4j               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPE2D+R3OOH=EPE3ooH2j               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPE2D+R3OOH=EPE2ooh3j               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPEED+R3OOH=EPEeoohmj               7.740e+03   2.29  1.108e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!EPEED+R3OOH=EPEmoohej               2.470e+04   2.13  1.216e+04   !Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012
!
!EPE5ooh3j=>EB3D+HCHO+R2OH             2.000e+13   0.00  2.870e+04   !
!EPE5ooh3j=>C2H5OCO+c4h81ooh3d       2.000e+13   0.00  2.870e+04   !
!EPE5ooH2j=>EP2d+R16C2H4OOH             2.000e+13   0.00  2.870e+04   !
!EPE4ooH2j=>EP2d+CH3CHO+R2OH           2.000e+13   0.00  2.870e+04   !
!EPE3ooh5j=>C2H4Z+EP3*o+R2OH            2.000e+13   0.00  2.870e+04   !
!EPE2ooh5j=>C2H4Z+EP2d+R3OOH          2.000e+13   0.00  2.870e+04   !
!EPE2ooh4j=>C3H6Y+ea2*o+R2OH            2.000e+13   0.00  2.870e+04   !
!EPE2oohej=>CH3CHO+C4H8CO+R3OOH      2.000e+13   0.00  2.870e+04   !
!EPEeooH2j=>CH3CHO+C4H8CO+R3OOH      2.000e+13   0.00  2.870e+04   !
!
!EPE5oo=EPE4D+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPE4oo=EPE4D+R3OOH                 5.075E+42  -9.410 4.249E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPE4oo=EPE3D+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPE3oo=EPE3D+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPE3oo=EPE2D+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
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!EPE2oo=EPE2D+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPEeoo=EPEED+R3OOH                 5.075E+42  -9.410 4.249E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EPEmoo=EPEED+R3OOH                 5.044E+38  -8.110 4.149E+04 !Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!
EPE5J=C2H4Z+EP3J                   2.000E+13   0.00  2.870E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
EPE4J=C3H6Y+EA2J                   5.250E+11   0.50    26591.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EPE4J=C3H6Y+EA2J                   2.000E+13   0.00  2.870E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
!EPE3J=C4H8Y+C2H5OCO              4.530E+12   0.335   34269.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
EPE3J=C4H8Y+C2H5OCO              2.000E+13   0.00  3.100E+04   !Dayma et
al.,Int J Chem Kinet, 35 (2003) 273-285
EPE3J=EB3D+R4CH3                   2.000E+13   0.00  3.100E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
!EPE2J=C4H8CO+R15C2H5O              2.786E+22  -2.31  4.566E+04
EPE2J=C4H8CO+R15C2H5O              1.460E+12   0.61    53276.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
EPE2J=R11C2H5   +EP2d                 2.000E+13   0.00  3.470e+04   !
Dayma et al.,Int J Chem Kinet, 35 (2003) 273-285 (+6kcal)
!EPE2J=R11C2H5   +EP2d                1.330E+11    0.97   34882.0 !Huynh
and Violi J.Org.Chem. 73 (2008) 94-101
!EPEEJ=CH3CHO+NC4H9CO              1.127E+21  -1.73  4.055E+04
EPEEJ=CH3CHO+NC4H9CO              1.127E+21  -1.73  4.255E+04   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EPEMJ=C2H4Z+C4H9CO2                2.325E+14  -0.20  3.297E+04
EPEMJ=C2H4Z+C4H9CO2                2.000E+13   0.00  2.800E+04
MPEMJ=HCHO+NC4H9CO                1.230E+13   0.375   36714.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101

EPE5J=EPE4D+R1H                     3.000e+13   0.00  3.800e+04  !ST
EPE4J=EPE4D+R1H                     3.000e+13   0.00  3.900e+04  !ST
EPE4J=EPE3D+R1H                     3.000e+13   0.00  3.800e+04  !ST
EPE3J=EPE3D+R1H                     3.000e+13   0.00  3.800e+04  !ST
EPE3J=EPE2D+R1H                     3.000e+13   0.00  3.800e+04  !ST
EPE2J=EPE2D+R1H                     3.000e+13   0.00  3.800e+04  !ST
EPEEJ=EPEED+R1H                     3.000e+13   0.00  3.900e+04  !ST
EPEMJ=EPEED+R1H                     3.000e+13   0.00  3.800e+04  !ST

C4H9COOH=>C4H8CO+H2O               4.470E+14   0.00  7.989E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C4H9COOH=>C4H10+CO2                7.080E+13   0.00  7.452E+04   !Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119
C4H9COOH=>NC4H9CO+R2OH              1.4E+0017   0.000  105815.7  ! UI 8
KB
C4H9COOH=>C4H9CO2+R1H               2.3E+0014   0.000  106345.3  ! UI 9
KB
C4H9COOH=>R20C4H9+HOCO              8.2E+0016   0.000   88817.0  ! UI 10
KB
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C4H9COOH=>R19C3H7+CH2COOH           2.9E+0016   0.000   78917.1  ! UI 11
KB
C4H9COOH=>R11C2H5   +CH2CH2COOH         1.7E+0017   0.000   87662.1  ! UI
12 KB

C4H9COOH+R1H=BUCOOH-5+H2            9.400e+04   2.75  6.280e+03   !2
anc7, primARy f
C4H9COOH+R1H=BUCOOH-4+H2            1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
C4H9COOH+R1H=BUCOOH-3+H2            1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
C4H9COOH+R1H=BUCOOH-2+H2            1.300E+06   2.4   4.471E+03   !2
anc7, secondARy
!C4H9COOH+R1H=BUCOOH-2+H2            5.400e+04   2.5  -1.900e+03   !
!C4H9COOH+R1H=C4H9CO2+H2             4.2E+0006   2.000    2400.0   ! ME
96 CN
C4H9COOH+R1H=C4H9CO2+H2             5.550E-23   10.60   -4459.0   !
PARk,Zhu,Lin, JcP 118, 9990-9996 (2003)
C4H9COOH+B1O=BUCOOH-5+R2OH           9.650e+04   2.68  3.716e+03   !2
anc7, primARy f
C4H9COOH+B1O=BUCOOH-4+R2OH           4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
C4H9COOH+B1O=BUCOOH-3+R2OH           4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
C4H9COOH+B1O=BUCOOH-2+R2OH           4.770E+04   2.71  2.106E+03   !2
anc7, secondARy
!C4H9COOH+B1O=BUCOOH-2+R2OH           8.800e+10   0.70  3.250e+03   !
!C4H9COOH+B1O=C4H9CO2+R2OH            1.0E+0013   0.000    3280.0   ! ME
87 CW
C4H9COOH+B1O=C4H9CO2+R2OH            1.460E-03    4.73    1727.0   ! Wu,
Lee, Xu, Lin, JPcA 2007
C4H9COOH+R2OH=BUCOOH-5+H2O          5.250e+09   0.97  1.590e+03   !2
rnc7, primARy;
C4H9COOH+R2OH=BUCOOH-4+H2O          4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
C4H9COOH+R2OH=BUCOOH-3+H2O          4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
C4H9COOH+R2OH=BUCOOH-2+H2O          4.680E+07   1.61 -3.500E+01   !2
rnc7, secondARy
!C4H9COOH+R2OH=BUCOOH-2+H2O           3.000e+06   2.00 -1.520e+03   !
!C4H9COOH+R2OH=C4H9CO2+H2O            1.1E+0006   2.000   -1865.0   ! ME
105 CW
C4H9COOH+R2OH=C4H9CO2+H2O           2.810E+02    2.97    -580.0   ! Xu
Lin pci 2007 31 159-166
C4H9COOH+R4CH3=BUCOOH-5+CH4         4.520e-01   3.65  7.154e+03   !2
anc7, primARy f
C4H9COOH+R4CH3=BUCOOH-4+CH4         2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
C4H9COOH+R4CH3=BUCOOH-3+CH4         2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
C4H9COOH+R4CH3=BUCOOH-2+CH4         2.705E+04   2.26  7.287E+03   !2
anc7, secondARy
!C4H9COOH+R4CH3=BUCOOH-2+CH4          1.000e+11   0.00  7.300e+03   !
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C4H9COOH+R4CH3=C4H9CO2+CH4          2.035E+00    3.57    7722.0   !
Xu,PARk,Lin, JcP 120, 6593-6599 (2004)
C4H9COOH+R3OOH=BUCOOH-5+H2O2        8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C4H9COOH+R3OOH=BUCOOH-4+H2O2        5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
C4H9COOH+R3OOH=BUCOOH-3+H2O2        5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
C4H9COOH+R3OOH=>BUCOOH-2+H2O2        5.600E+12   0.00  1.769E+04   !2
anc7, secondARy
!C4H9COOH+R3OOH=BUCOOH-2+H2O2        6.400e+03   2.60  1.240e+04   !
!C4H9COOH+R3OOH=C4H9CO2+H2O2         2.11E+0006  0.000   14000.0   ! ME
96 CN
C4H9COOH+R3OOH=C4H9CO2+H2O2         2.500E+12    0.00   24000.0 ! MARinov
1998
C4H9COOH+R8CH3OO=BUCOOH-5+CH3OOH    8.400e+12   0.00  2.044e+04   !2
anc7, primARy f
C4H9COOH+R8CH3OO=BUCOOH-4+CH3OOH    5.600E+12   0.00  1.769E+04   !2
corrected to ag
C4H9COOH+R8CH3OO=BUCOOH-3+CH3OOH    5.600E+12   0.00  1.769E+04   !2
corrected to ag
C4H9COOH+R8CH3OO=BUCOOH-2+CH3OOH    5.600E+12   0.00  1.769E+04   !2
corrected to ag
!C4H9COOH+R8CH3OO=BUCOOH-2+CH3OOH    6.400e+03   2.60  1.240e+04   !
C4H9COOH+R7CH3O  =BUCOOH-5+CH3OH      1.581e+11   0.00  7.000e+03   !2
rnc7, primARy;
C4H9COOH+R7CH3O  =BUCOOH-4+CH3OH      1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
C4H9COOH+R7CH3O  =BUCOOH-3+CH3OH      1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
C4H9COOH+R7CH3O  =BUCOOH-2+CH3OH      1.095E+11   0.00  5.000E+03   !2
anc7, secondARy
!C4H9COOH+R7CH3O  =BUCOOH-2+CH3OH      1.780e+12   0.00  1.200e+03   !

BUCOOH-5=C2H4Z+CH2CH2COOH          2.000E+13   0.00  2.870E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
BUCOOH-4=C3H6Y+CH2COOH             5.250E+11   0.50    26591.0   !Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!BUCOOH-4=C3H6Y+CH2COOH             2.000E+13   0.00  2.870E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
BUCOOH-3=C4H8Y+HOCO              3.030E+13   0.27    34667.0   !Huynh and
Violi J.Org.Chem. 73 (2008) 94-101
!BUCOOH-3=C4H8Y+HOCO             4.217E+14  -0.32  3.486E+04
BUCOOH-3=>C3H5COOH+R4CH3            2.000E+13   0.00  3.100E+04   !Dayma
et al.,Int J Chem Kinet, 35 (2003) 273-285
BUCOOH-2=C4H8CO+R2OH             3.046E+21  -1.61  5.730E+04
BUCOOH-2=R11C2H5   +C2H3COOH           2.000E+13   0.00  3.270e+04   !
Dayma et al.,Int J Chem Kinet, 35 (2003) 273-285 (+4kcal)
BUCOOH-2=>CO2+R20C4H9          1.700E+09   1.0     38640.0
C4H9CO2+m=R20C4H9+CO2+m             4.400E+15   0.00  1.050E+04
C3H7COCO2+m=>NC3H7CO+CO2+m        4.400E+15    0.00   10500.0
CH3COCO2+m=>R14CH3CO+CO2+m          4.400E+15    0.00   10500.0
NC4H9CO=>R20C4H9+B2CO                1.834e+15  -0.73  1.291e+04   !
Glaude et al., DMC C2H5CO
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BUCOOH-5=C4H7COOH+R1H                3.000E+13   0.00    38000.0   !ST
BUCOOH-4=C4H7COOH+R1H                3.000E+13   0.00    38000.0   !ST
BUCOOH-3=C4H7COOH+R1H                3.200E+13   0.00    34800.0   !ST
BUCOOH-2=C4H7COOH+R1H                3.000E+13   0.00  5.150E+04   !ST
C4H7COOH+R2OH=>HCHO+PRCOOH-4         1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C4H7COOH+R2OH=>CH3CHO+CH2CH2COOH     1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C4H7COOH+R2OH=>C2H5CHO+CH2COOH       1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
C4H7COOH+R1H=>H2+CO2+C4H7-1          4.2E+0006  2.100     6900.0   ! MZB
483
C4H7COOH+R2OH=>H2O+CO2+C4H7-1        5.4E+0004  2.000     -340.0   ! MZB
484
C4H7COOH+R3OOH=>H2O2+CO2+C4H7-1      1.0E+0011  0.000    11500.0   ! MZB
485
C4H7COOH+R4CH3=>CH4+CO2+C4H7-1       1.4E+0001  3.100     9940.0   ! MZB
486
C4H7COOH+R11C2H5   =>C2H6+CO2+C4H7-1    1.4E+0001  3.100     8940.0   !
MZB 487
EPE4D+R2OH=>HCHO+EB4J                1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPE4D+R2OH=>CH3CHO+EP3J              1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPE3D+R2OH=>CH3CHO+EP3J              1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPE3D+R2OH=>C2H5CHO+EA2J             1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPE2D+R2OH=>C2H5CHO+EA2J             1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPEED+R2OH=>HCHO+MPEMJ               1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPEED+R2OH=>CH3CHO+C4H9CO2           1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EPE4D=C4H7COOH+C2H4Z                 2.000E+12   0.00  4.729E+04
EPE3D=C4H7COOH+C2H4Z                 2.000E+12   0.00  4.729E+04
EPE2D=C4H7COOH+C2H4Z                 2.000E+12   0.00  4.729E+04
!EPE2D(+m)=C4H7COOH+C2H4Z(+m)        4.000E+12   0.00  5.000E+04
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off
reaction
!END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CH3CO2+M=R4CH3+CO2+M                       4.400E+15    0.00   10500.0
!!!!!!!!!!!!!!!!!Reactions of propanal!!!!!!!!!!!!!!!!!
!C2H5CHO=R13CH2CHO+R4CH3                   1.000e+17   0.0   8.465e+04   !
asC4H10 Dean, J.Phys.Chem. 89 (1985) 4600-4608
!C4H8Y+R2OH=R4CH3+C2H5CHO          6.800E+11   0.0    -928.0 !(89ATK*RTi)
!metathesis same as n-butanal
C2H5CHO+R3OOH=R25C2H5CO+H2O2             1.700E+12    0.00   10700.0 !
(COLKET 77; C
C2H5CHO+R2OH=CH3CHCHO+H2O             4.680e+07   1.61 -3.500e+01   !2
rnc7, se
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!C2H5CHO+R2OH=R25C2H5CO+H2O               2.650E+12   0.00     -730.0   !
Atkinson et
!C2H5CHO+R1H=R25C2H5CO+H2                 1.200E+14   0.00     7000.0   !
Yasunaga et
!decomposition
R25C2H5CO=CH3CHCO+R1H                    4.658E+10   0.79  4.255E+04   !
rev / 2.000
R25C2H5CO=CH2COZ  +R4CH3                    2.745E+09   1.41
3.583E+04   !rev / 1.
!R25C2H5CO=>R11C2H5+B2CO                     1.834e+15  -0.73  1.291e+04
!Glaude et a
CH3CHCHO=CH3CHCO+R1H 1.345E+13 -0.17 3.346E+04
          rev / 5.000E+12 0.00 1.200E+03 /
!!!!!!!!!!Reactions of butanal!!!!!!!!!
!initiation
NC3H7CHO=R11C2H5+R13CH2CHO        1.580e+17   0.0   8.028e+04   !asC4H10
Dean, J.Phys.Chem. 89 (1985) 4600-4608
!metathesis
NC3H7CHO+R1H=NC3H7CO+H2                1.200E+14   0.00     7000.0   !
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!decomposition
NC3H7CO+M=R19C3H7+B2CO+M                      8.640E+15    0.00
14400.0 !(WILK89) idem R14CH3CO+M
NC3H7CO=CH2COZ  +R11C2H5         2.745E+09   1.41  3.583E+04 !
rev / 1.000E+04   2.48  6.130E+03 /
END
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